



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 09:04 AM EDT

PDB ID : 9Q3Q / pdb_00009q3q
EMDB ID : EMD-72204
Title : Cryo-EM structure of translating Escherichia coli 70S ribosome bound to mRNA, P-site QKF-peptidyl-tRNAPhe, glycyl-tRNAGly in A/T conformation, EF-Tu-GDP, and bottromycin at 2.01Å resolution
Authors : Travin, D.Y.; Basu, R.S.; Paranjpe, M.; Klepacki, D.; Zhurakovskaya, A.I.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.; Gagnon, M.G.
Deposited on : 2025-08-19
Resolution : 2.01 Å(reported)
Based on initial model : 8G7P

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

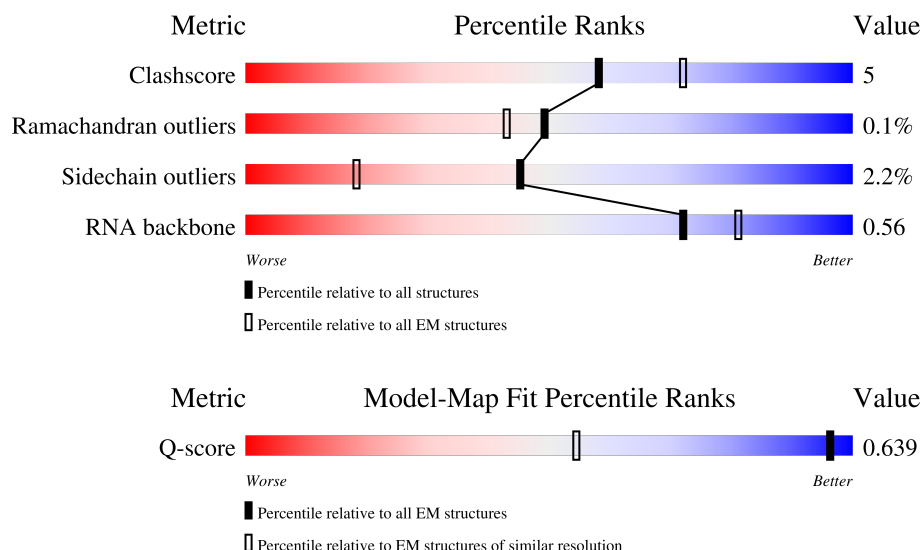
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



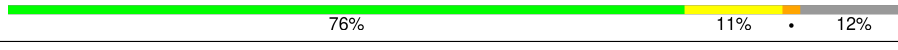
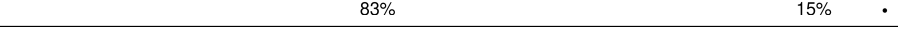
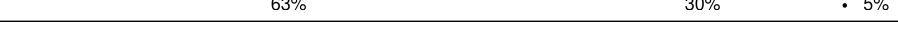
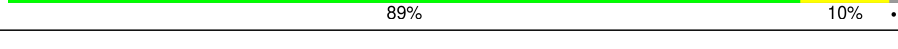
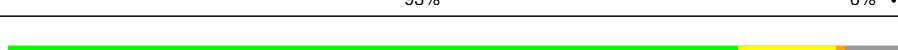
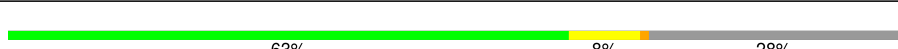
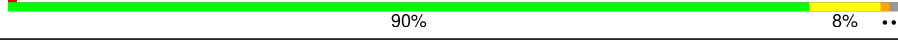
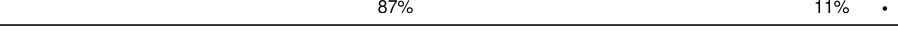
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1691 (1.52 - 2.51)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1542	

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Mol	Chain	Length	Quality of chain
2	b	241	
3	c	233	
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	101	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	v	45	
23	w	76	
24	x	76	
25	y	3	
26	z	394	

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Mol	Chain	Length	Quality of chain
27	A	2904	
28	B	120	
29	C	273	
30	D	209	
31	E	201	
32	F	179	
33	G	177	
34	H	149	
35	J	142	
36	L	142	
37	M	123	
38	N	144	
39	O	136	
40	P	127	
41	Q	117	
42	R	115	
43	S	118	
44	T	103	
45	U	110	
46	V	100	
47	W	104	
48	X	94	
49	Y	85	
50	Z	78	
51	1	63	

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Mol	Chain	Length	Quality of chain
52	2	59	81% 15%
53	3	70	61% 24% 14%
54	4	57	82% 14%
55	5	55	87% 7%
56	6	46	91% 9%
57	7	65	89% 9%
58	8	38	97%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 151192 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1529	Total	C	N	O	P	0	0
			32825	14647	6024	10625	1529		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1754	1110	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A7ZSI6

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called dapG mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	11	Total	C	N	O	P	0	0
			239	106	45	77	11		

- Molecule 23 is a RNA chain called A/T-site glycine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	74	Total	C	N	O	P	0	0
			1588	708	283	523	74		

- Molecule 24 is a RNA chain called P-site phenylalanine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	x	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

- Molecule 25 is a protein called QKF peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	y	3	Total	C	N	O	0	0
			29	20	5	4		

- Molecule 26 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	z	371	Total	C	N	O	S	0	0
			2876	1823	492	548	13		

- Molecule 27 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 28 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 34 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 35 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	O	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Q	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	S	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	W	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	X	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Y	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Z	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	60	Total	C	N	O	S	0	0
			476	296	89	85	6		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 56 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	46	Total	C	N	O	S	0	0
			373	225	89	57	2		

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 58 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	a	150	Total	Mg	0
			150	150	
59	d	1	Total	Mg	0
			1	1	
59	j	1	Total	Mg	0
			1	1	
59	l	1	Total	Mg	0
			1	1	
59	x	1	Total	Mg	0
			1	1	
59	A	656	Total	Mg	0
			656	656	
59	B	2	Total	Mg	0
			2	2	
59	C	18	Total	Mg	0
			18	18	
59	D	7	Total	Mg	0
			7	7	

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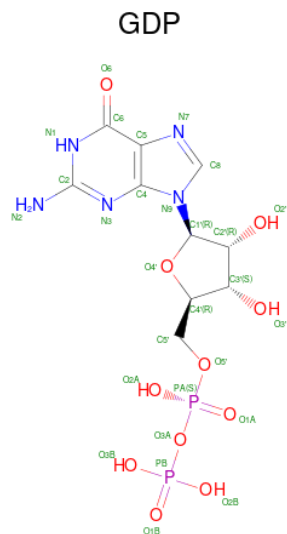
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Mol	Chain	Residues	Atoms		AltConf
59	E	2	Total 2	Mg 2	0
59	N	2	Total 2	Mg 2	0
59	O	1	Total 1	Mg 1	0
59	R	1	Total 1	Mg 1	0
59	S	3	Total 3	Mg 3	0
59	2	1	Total 1	Mg 1	0
59	4	7	Total 7	Mg 7	0
59	6	3	Total 3	Mg 3	0
59	7	1	Total 1	Mg 1	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

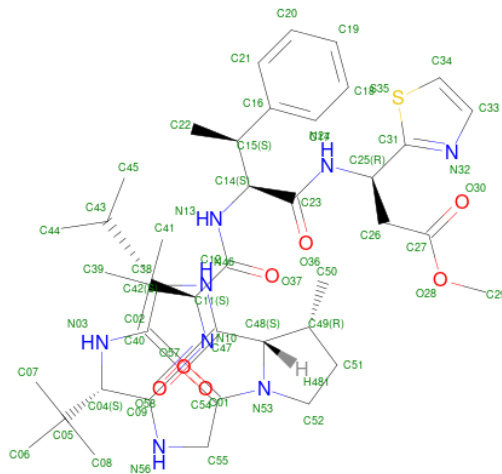
Mol	Chain	Residues	Atoms		AltConf
60	a	30	Total 30	K 30	0
60	f	1	Total 1	K 1	0
60	A	89	Total 89	K 89	0
60	B	1	Total 1	K 1	0
60	C	1	Total 1	K 1	0
60	D	1	Total 1	K 1	0
60	E	1	Total 1	K 1	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
61	z	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 62 is Bottromycin A2 (CCD ID: MQH) (formula: $C_{42}H_{62}N_8O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
62	z	1	Total 58	C 42	N 8	O 7	S 1	0

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	3	1	Total 1	Zn 1	0
63	8	1	Total 1	Zn 1	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	a	294	Total 294	O 294	0
64	k	3	Total 3	O 3	0
64	l	4	Total 4	O 4	0
64	s	1	Total 1	O 1	0
64	v	4	Total 4	O 4	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	A	1365	Total 1365	O 1365	0
64	B	12	Total 12	O 12	0
64	C	36	Total 36	O 36	0
64	D	12	Total 12	O 12	0
64	E	17	Total 17	O 17	0
64	M	1	Total 1	O 1	0
64	N	11	Total 11	O 11	0
64	O	3	Total 3	O 3	0
64	P	5	Total 5	O 5	0
64	R	2	Total 2	O 2	0
64	S	3	Total 3	O 3	0

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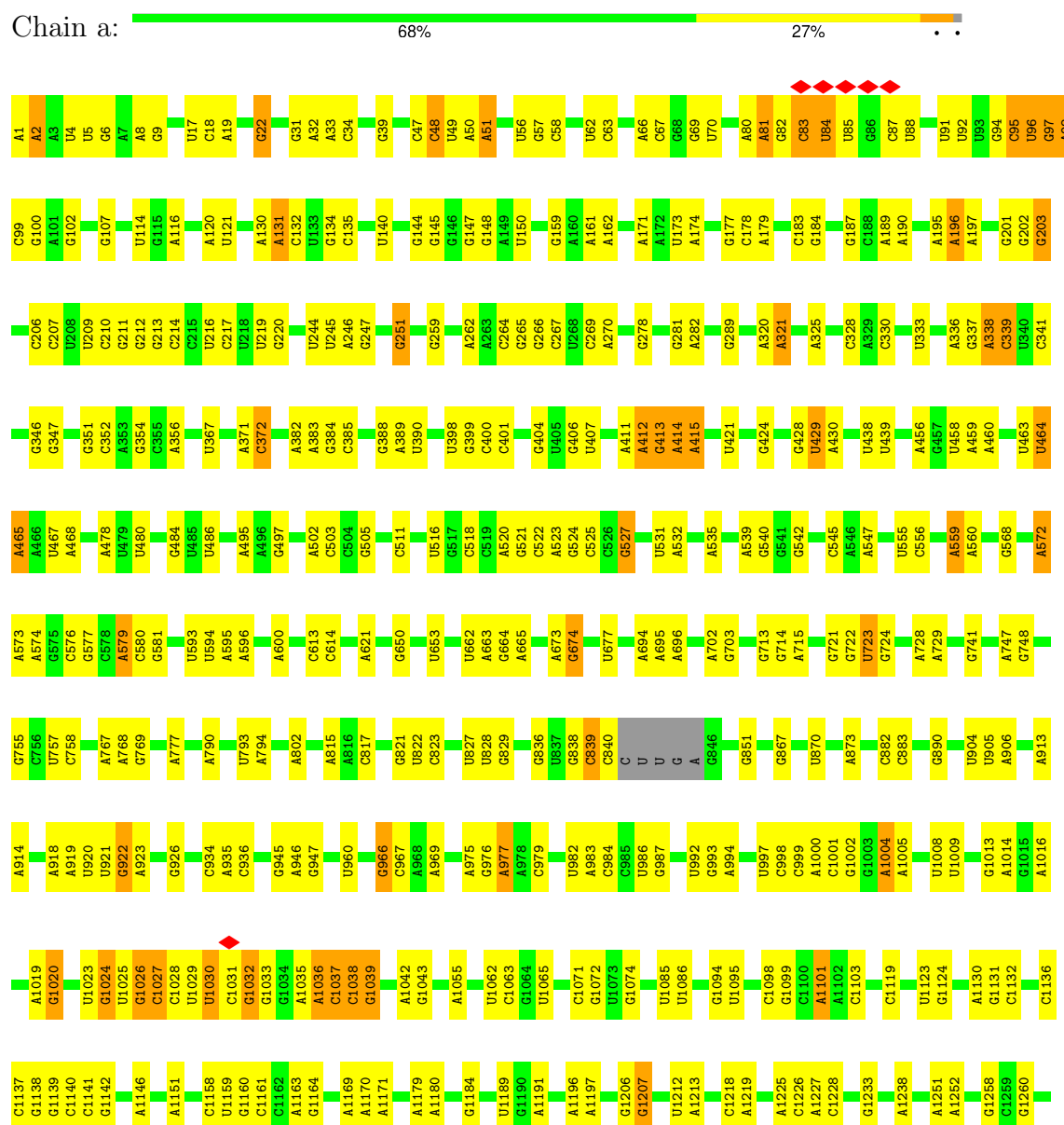
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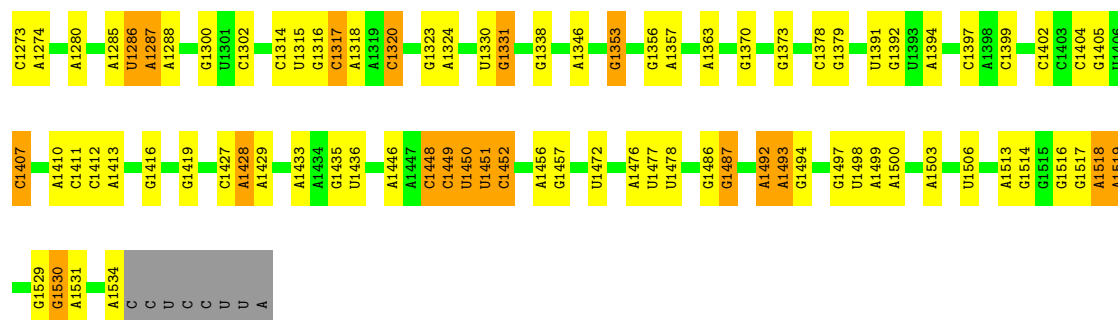
Mol	Chain	Residues	Atoms		AltConf
64	T	1	Total 1	O 1	0
64	U	5	Total 5	O 5	0
64	V	1	Total 1	O 1	0
64	X	1	Total 1	O 1	0
64	Y	1	Total 1	O 1	0
64	Z	1	Total 1	O 1	0
64	4	11	Total 11	O 11	0
64	6	4	Total 4	O 4	0
64	7	7	Total 7	O 7	0
64	8	1	Total 1	O 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

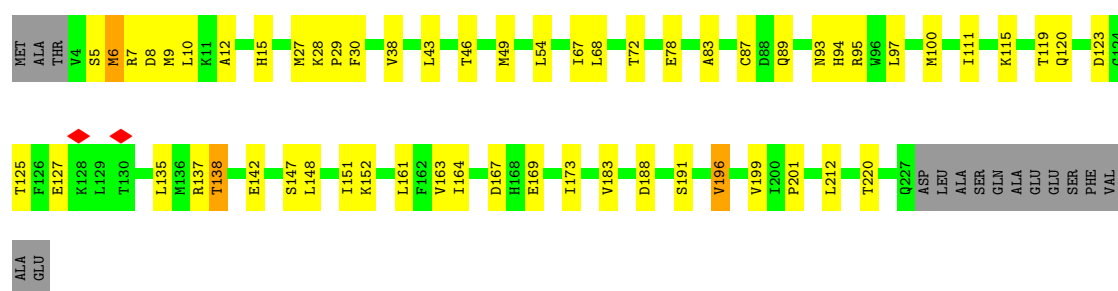
• Molecule 1: 16S Ribosomal RNA





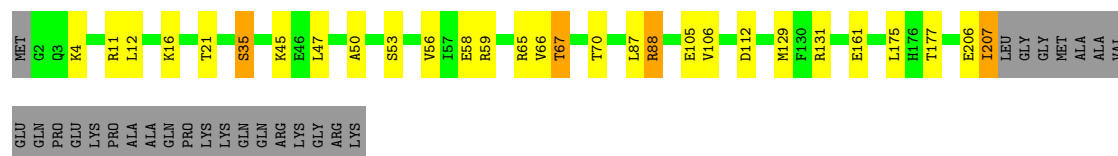
• Molecule 2: 30S ribosomal protein S2

Chain b: 69% 23% 7%



• Molecule 3: Small ribosomal subunit protein uS3

Chain c: 76% 11% 12%



• Molecule 4: Small ribosomal subunit protein uS4

Chain d: 83% 15%



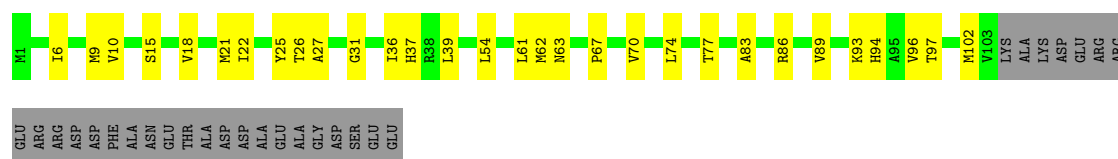
• Molecule 5: Small ribosomal subunit protein uS5

Chain e: 81% 13% 7%

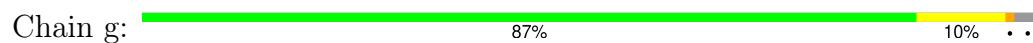


• Molecule 6: 30S ribosomal protein S6

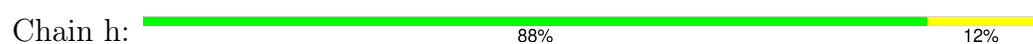
Chain f: 56% 23% 21%



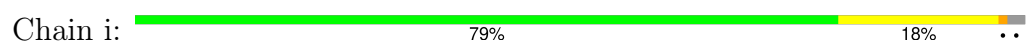
- Molecule 7: 30S ribosomal protein S7



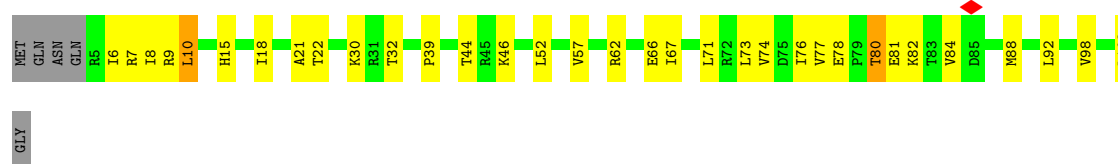
- Molecule 8: Small ribosomal subunit protein uS8



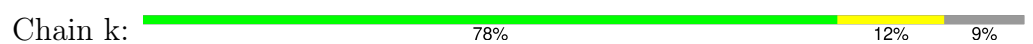
- Molecule 9: Small ribosomal subunit protein uS9



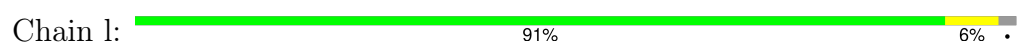
- Molecule 10: Small ribosomal subunit protein uS10



- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12





- Molecule 13: Small ribosomal subunit protein uS13

Chain m: 89% 8%



- Molecule 14: Small ribosomal subunit protein uS14

Chain n: 86% 13%



- Molecule 15: Small ribosomal subunit protein uS15

Chain o: 89% 10%



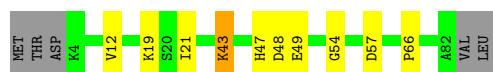
- Molecule 16: Small ribosomal subunit protein bS16

Chain p: 93% 6%



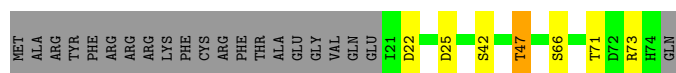
- Molecule 17: Small ribosomal subunit protein uS17

Chain q: 82% 11% 6%



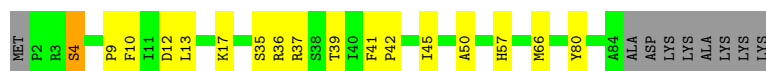
- Molecule 18: Small ribosomal subunit protein bS18

Chain r: 63% 8% 28%

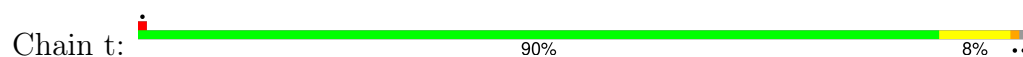


- Molecule 19: Small ribosomal subunit protein uS19

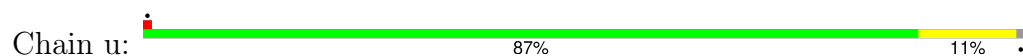
Chain s: 72% 17% 10%



- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein bS21



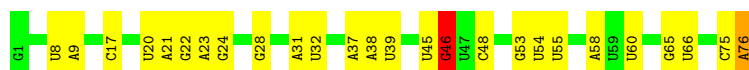
- Molecule 22: dapG mRNA



- Molecule 23: A/T-site glycine tRNA



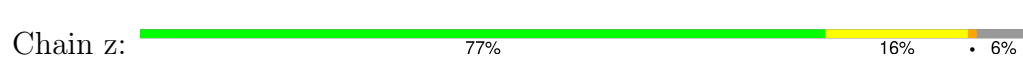
- Molecule 24: P-site phenylalanine tRNA

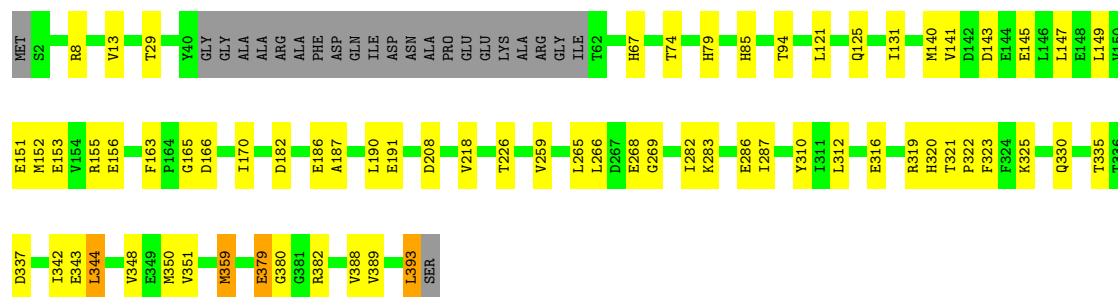


- Molecule 25: QKF peptide



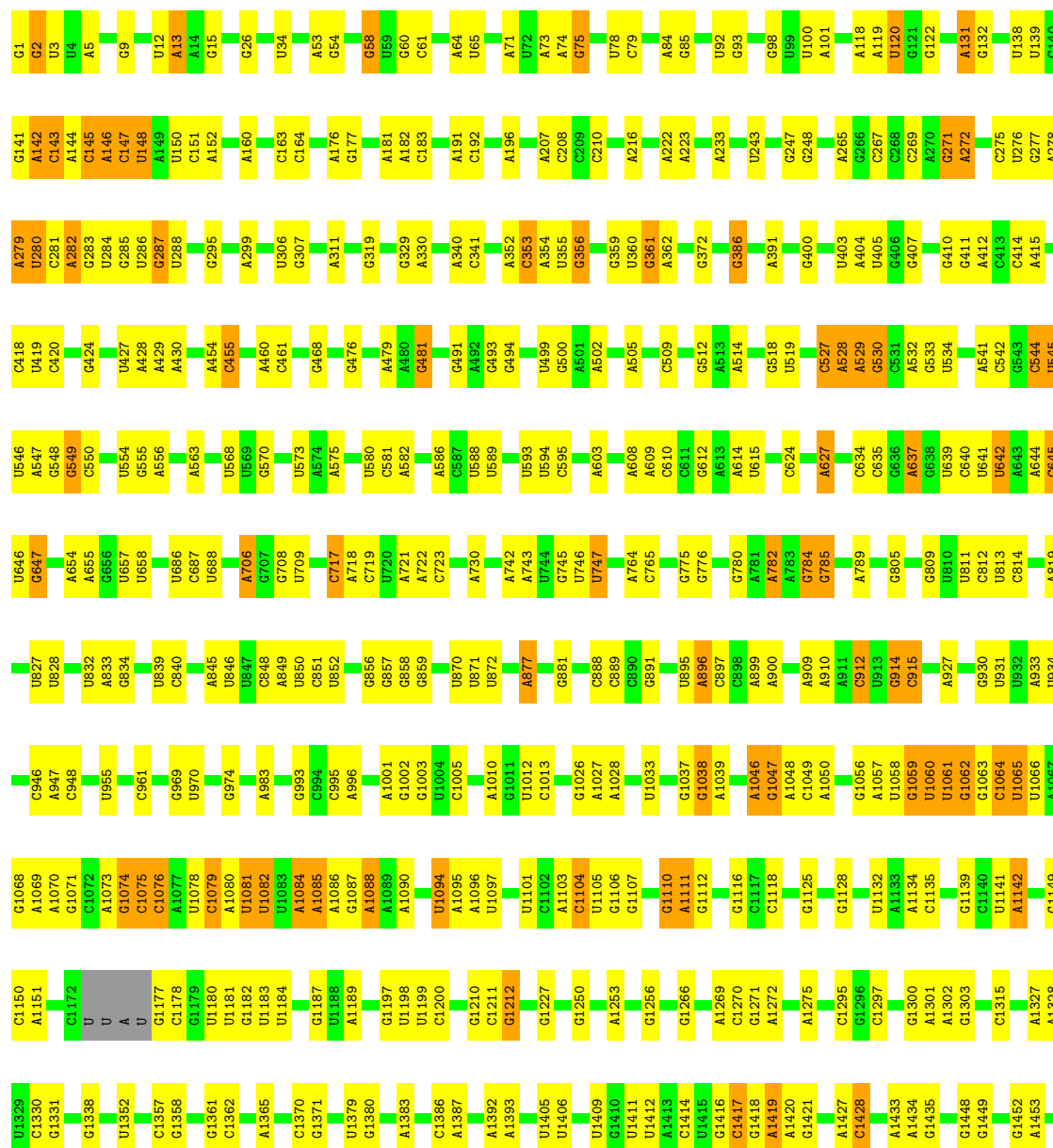
- Molecule 26: Elongation factor Tu 2





• Molecule 27: 23S Ribosomal RNA

Chain A: 68% 27% 5%



Chain C:  90% 10%



- Molecule 30: 50S ribosomal protein L3

Chain D:  90% 10%



- Molecule 31: Large ribosomal subunit protein uL4

Chain E:  87% 12%



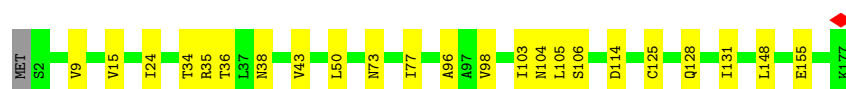
- Molecule 32: Large ribosomal subunit protein uL5

Chain F:  84% 15%



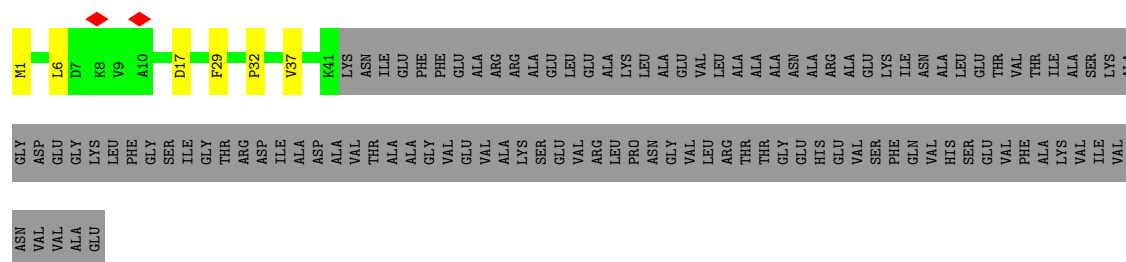
- Molecule 33: Large ribosomal subunit protein uL6

Chain G:  86% 13%



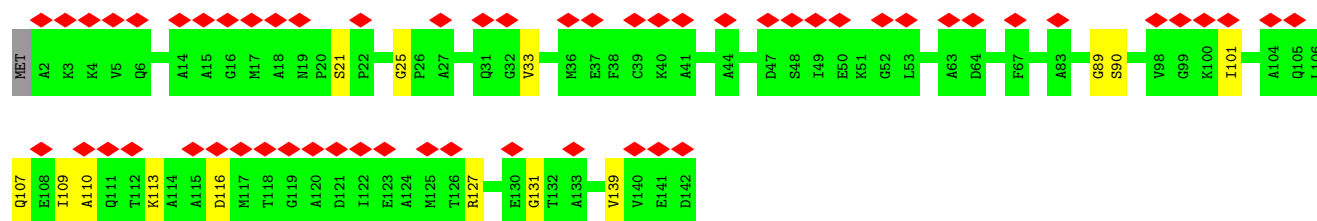
- Molecule 34: Large ribosomal subunit protein bL9

Chain H:  23% 72%



- Molecule 35: 50S ribosomal protein L11

Chain J:  40% 89% 10%



- Molecule 36: Large ribosomal subunit protein uL13

Chain L: 94% 6%



- Molecule 37: Large ribosomal subunit protein uL14

Chain M: 90% 10%



- Molecule 38: 50S ribosomal protein L15

Chain N: 89% 11%



- Molecule 39: Large ribosomal subunit protein uL16

Chain O: 86% 14%



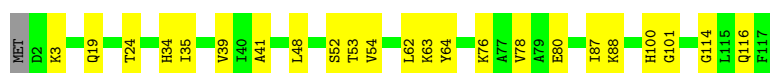
- Molecule 40: Large ribosomal subunit protein bL17

Chain P: 84% 9% 7%



- Molecule 41: Large ribosomal subunit protein uL18

Chain Q: 79% 20%



- Molecule 42: Large ribosomal subunit protein bL19

Chain R:  91% 8%



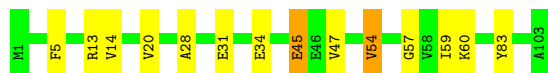
- Molecule 43: 50S ribosomal protein L20

Chain S:  92% 8%



- Molecule 44: Large ribosomal subunit protein bL21

Chain T:  86% 12%



- Molecule 45: Large ribosomal subunit protein uL22

Chain U:  93% 7%



- Molecule 46: 50S ribosomal protein L23

Chain V:  86% 7% 7%



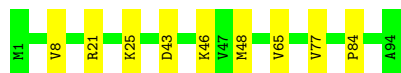
- Molecule 47: 50S ribosomal protein L24

Chain W:  80% 17%

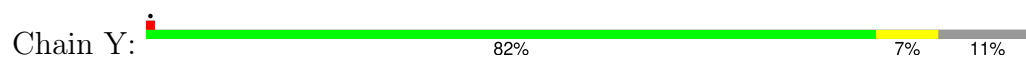


- Molecule 48: Large ribosomal subunit protein bL25

Chain X:  90% 10%



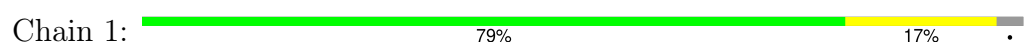
- Molecule 49: 50S ribosomal protein L27



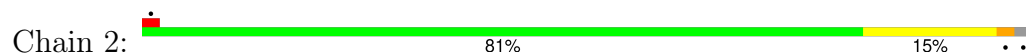
- Molecule 50: 50S ribosomal protein L28



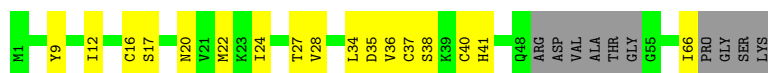
- Molecule 51: Large ribosomal subunit protein uL29



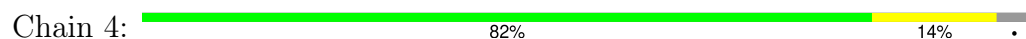
- Molecule 52: 50S ribosomal protein L30



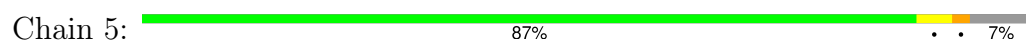
- Molecule 53: 50S ribosomal protein L31



- Molecule 54: 50S ribosomal protein L32



- Molecule 55: 50S ribosomal protein L33



- Molecule 56: Large ribosomal subunit protein bL34

Chain 6:  91% 9%



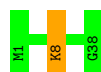
- Molecule 57: 50S ribosomal protein L35

Chain 7:  89% 9% .



- Molecule 58: Large ribosomal subunit protein bL36A

Chain 8:  97% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	375097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.463	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.559	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	425.9328, 425.9328, 425.9328	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8319, 0.8319, 0.8319	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1CNX, 3TD, H2U, 2MG, MG, OMC, 1MG, 4D4, IAS, 4SU, GDP, 4OC, MIA, OMU, MS6, UR3, 5MU, 5MC, K, MEQ, ZN, 6MZ, PSU, 2MA, OMG, G7M, MQH, MA6, D2T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.33	0/36475	0.37	0/56895
2	b	0.19	0/1785	0.36	0/2404
3	c	0.24	0/1651	0.36	0/2225
4	d	0.22	0/1665	0.33	0/2227
5	e	0.27	0/1165	0.40	0/1568
6	f	0.25	0/858	0.43	0/1160
7	g	0.21	0/1206	0.35	0/1617
8	h	0.22	0/989	0.34	0/1326
9	i	0.24	0/1034	0.36	0/1375
10	j	0.23	0/796	0.40	0/1077
11	k	0.22	0/884	0.35	0/1191
12	l	0.28	0/945	0.39	0/1268
13	m	0.21	0/900	0.34	0/1204
14	n	0.24	0/817	0.33	0/1088
15	o	0.21	0/722	0.32	0/964
16	p	0.25	0/653	0.39	0/877
17	q	0.22	0/650	0.35	0/871
18	r	0.24	0/453	0.37	0/609
19	s	0.23	0/680	0.33	0/915
20	t	0.24	0/676	0.38	0/895
21	u	0.21	0/597	0.32	0/792
22	v	0.33	0/267	0.36	0/415
23	w	0.31	1/1626 (0.1%)	0.36	0/2528
24	x	0.32	1/1651 (0.1%)	0.36	0/2569
25	y	0.22	0/29	0.61	0/36
26	z	0.21	0/2929	0.38	0/3964
27	A	0.38	0/69147	0.41	1/107869 (0.0%)
28	B	0.29	0/2876	0.36	0/4483
29	C	0.27	0/2121	0.37	0/2852
30	D	0.27	0/1576	0.35	0/2119
31	E	0.25	0/1571	0.37	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	F	0.20	0/1434	0.33	0/1926
33	G	0.21	0/1343	0.34	0/1816
34	H	0.24	0/306	0.50	0/413
35	J	0.13	0/692	0.33	0/960
36	L	0.26	0/1152	0.34	0/1551
37	M	0.27	0/955	0.38	0/1279
38	N	0.26	0/1061	0.36	0/1412
39	O	0.26	0/1073	0.37	0/1433
40	P	0.26	0/958	0.34	0/1281
41	Q	0.21	0/902	0.36	0/1209
42	R	0.26	0/929	0.35	0/1242
43	S	0.26	0/960	0.34	0/1278
44	T	0.27	0/829	0.36	0/1107
45	U	0.27	0/864	0.34	0/1156
46	V	0.24	0/744	0.36	0/994
47	W	0.24	0/787	0.41	0/1051
48	X	0.23	0/766	0.37	0/1025
49	Y	0.24	0/587	0.34	0/776
50	Z	0.26	0/635	0.35	0/848
51	1	0.24	0/496	0.43	0/660
52	2	0.24	0/453	0.35	0/605
53	3	0.21	0/484	0.35	0/645
54	4	0.27	0/440	0.36	0/588
55	5	0.22	0/424	0.37	0/565
56	6	0.26	0/376	0.38	0/494
57	7	0.33	0/513	0.44	0/676
58	8	0.30	0/303	0.32	0/397
All	All	0.33	2/159860 (0.0%)	0.39	1/238883 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	w	46	G7M	O3'-P	6.82	1.63	1.56
24	x	8	4SU	O3'-P	5.03	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	512	G	O4'-C1'-N9	5.47	116.40	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32825	0	16531	227	0
2	b	1754	0	1782	39	0
3	c	1624	0	1696	15	0
4	d	1643	0	1707	24	0
5	e	1152	0	1196	14	0
6	f	839	0	833	16	0
7	g	1191	0	1245	8	0
8	h	979	0	1031	9	0
9	i	1022	0	1070	16	0
10	j	786	0	828	23	0
11	k	877	0	883	12	0
12	l	942	0	999	5	0
13	m	891	0	952	7	0
14	n	805	0	844	10	0
15	o	714	0	734	5	0
16	p	643	0	661	2	0
17	q	641	0	682	6	0
18	r	446	0	472	4	0
19	s	663	0	688	15	0
20	t	670	0	719	5	0
21	u	589	0	629	7	0
22	v	239	0	119	1	0
23	w	1588	0	798	17	0
24	x	1632	0	837	7	0
25	y	29	0	29	2	0
26	z	2876	0	2898	47	0
27	A	62252	0	31312	449	0
28	B	2572	0	1301	34	0
29	C	2082	0	2153	16	0
30	D	1566	0	1618	10	0
31	E	1552	0	1619	18	0
32	F	1410	0	1444	18	0
33	G	1323	0	1371	10	0
34	H	303	0	327	3	0
35	J	693	0	344	8	0
36	L	1129	0	1162	9	0
37	M	946	0	1023	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	1052	0	1127	10	0
39	O	1075	0	1145	11	0
40	P	945	0	989	8	0
41	Q	892	0	923	11	0
42	R	917	0	962	4	0
43	S	947	0	1019	8	0
44	T	816	0	839	9	0
45	U	857	0	922	4	0
46	V	738	0	807	6	0
47	W	779	0	831	11	0
48	X	753	0	780	4	0
49	Y	580	0	594	4	0
50	Z	625	0	652	3	0
51	1	495	0	526	8	0
52	2	449	0	488	7	0
53	3	476	0	467	9	0
54	4	434	0	445	5	0
55	5	417	0	451	3	0
56	6	373	0	407	3	0
57	7	504	0	572	5	0
58	8	302	0	340	1	0
59	2	1	0	0	0	0
59	4	7	0	0	0	0
59	6	3	0	0	0	0
59	7	1	0	0	0	0
59	A	656	0	0	0	0
59	B	2	0	0	0	0
59	C	18	0	0	0	0
59	D	7	0	0	0	0
59	E	2	0	0	0	0
59	N	2	0	0	0	0
59	O	1	0	0	0	0
59	R	1	0	0	0	0
59	S	3	0	0	0	0
59	a	150	0	0	0	0
59	d	1	0	0	0	0
59	j	1	0	0	0	0
59	l	1	0	0	0	0
59	x	1	0	0	0	0
60	A	89	0	0	0	0
60	B	1	0	0	0	0
60	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	D	1	0	0	0	0
60	E	1	0	0	0	0
60	a	30	0	0	0	0
60	f	1	0	0	0	0
61	z	28	0	12	0	0
62	z	58	0	0	2	0
63	3	1	0	0	0	0
63	8	1	0	0	0	0
64	4	11	0	0	0	0
64	6	4	0	0	0	0
64	7	7	0	0	0	0
64	8	1	0	0	0	0
64	A	1365	0	0	5	0
64	B	12	0	0	0	0
64	C	36	0	0	0	0
64	D	12	0	0	0	0
64	E	17	0	0	0	0
64	M	1	0	0	0	0
64	N	11	0	0	0	0
64	O	3	0	0	0	0
64	P	5	0	0	0	0
64	R	2	0	0	0	0
64	S	3	0	0	0	0
64	T	1	0	0	0	0
64	U	5	0	0	0	0
64	V	1	0	0	0	0
64	X	1	0	0	0	0
64	Y	1	0	0	0	0
64	Z	1	0	0	0	0
64	a	294	0	0	3	0
64	k	3	0	0	1	0
64	l	4	0	0	0	0
64	s	1	0	0	0	0
64	v	4	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
All	All	151192	0	99835	1152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1915:3TD:C1'	27:A:1915:3TD:O4'	1.65	1.17
28:B:8:C:O2'	28:B:9:G:O5'	1.76	1.03
27:A:1084:A:O2'	27:A:1085:A:O5'	1.79	0.99
27:A:2304:G:OP1	32:F:121:SER:OG	1.85	0.95
21:u:31:GLU:OE2	21:u:35:ARG:NE	2.00	0.94
10:j:80:THR:OG1	10:j:82:LYS:NZ	2.01	0.94
23:w:18:G:O2'	23:w:57:G:N2	2.03	0.91
1:a:96:U:O2'	1:a:97:G:O5'	1.89	0.90
27:A:12:U:O2'	27:A:13:A:O5'	1.89	0.90
50:Z:43:GLU:OE1	50:Z:45:ARG:NH1	2.05	0.90
1:a:1314:C:OP2	19:s:4:SER:OG	1.91	0.88
27:A:2178:C:O2'	27:A:2179:C:OP1	1.91	0.87
27:A:1085:A:O2'	27:A:1086:A:O4'	1.91	0.87
2:b:93:ASN:OD1	2:b:94:HIS:ND1	2.09	0.86
1:a:84:U:O4	1:a:88:U:O2'	1.94	0.86
2:b:120:GLN:OE1	2:b:137:ARG:NH1	2.11	0.84
27:A:1110:G:O2'	27:A:1111:A:O4'	1.95	0.83
1:a:673:A:O2'	1:a:674:G:OP1	1.97	0.82
1:a:159:G:N2	1:a:162:A:OP2	2.13	0.82
41:Q:114:GLY:O	41:Q:116:GLN:NE2	2.12	0.81
27:A:1721:G:O2'	27:A:1739:A:N6	2.13	0.81
27:A:1509:A:O2'	27:A:1510:G:O5'	1.98	0.80
52:2:4:THR:OG1	52:2:37:GLU:OE2	2.00	0.80
27:A:2134:A:N6	27:A:2157:G:O2'	2.14	0.80
27:A:534:U:O2'	43:S:49:ASP:OD2	2.00	0.79
35:J:127:ARG:O	35:J:131:GLY:N	2.14	0.79
1:a:333:U:OP1	20:t:2:ALA:N	2.16	0.79
27:A:1086:A:O2'	27:A:1103:A:N1	2.16	0.78
1:a:339:C:OP2	37:M:98:ARG:NH1	2.16	0.78
26:z:226:THR:OG1	26:z:282:ILE:O	2.02	0.78
1:a:81:A:O2'	1:a:82:G:O4'	2.00	0.78
19:s:12:ASP:OD1	19:s:35:SER:OG	2.01	0.77
30:D:42:ASN:ND2	30:D:43:ASP:OD1	2.17	0.77
1:a:203:G:O2'	1:a:465:A:N1	2.18	0.77
27:A:2128:G:N2	27:A:2173:A:O4'	2.17	0.77
14:n:49:GLN:NE2	19:s:12:ASP:OD2	2.18	0.76
1:a:202:G:O2'	1:a:468:A:N3	2.18	0.75
1:a:664:G:H22	1:a:741:G:H1	1.32	0.75
2:b:46:THR:OG1	2:b:201:PRO:O	2.04	0.75
23:w:9:A:O2'	23:w:10:G:N7	2.19	0.75
27:A:1418:G:O2'	27:A:1579:A:N6	2.20	0.74
27:A:2027:G:H1	27:A:2036:C:H5	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:146:A:O2'	27:A:147:C:OP2	2.05	0.74
15:o:17:ARG:NH1	15:o:18:ASP:OD2	2.21	0.73
55:5:5:ILE:HG23	55:5:28:ARG:NH2	2.03	0.73
19:s:10:PHE:O	19:s:39:THR:HG22	1.88	0.73
1:a:1005:A:N6	1:a:1024:G:N2	2.36	0.73
28:B:8:C:HO2'	28:B:9:G:P	2.12	0.73
27:A:2042:A:N3	64:A:3801:HOH:O	2.20	0.73
32:F:18:THR:OG1	32:F:19:GLU:OE1	2.06	0.72
51:1:51:ALA:O	51:1:55:THR:HG23	1.89	0.72
27:A:627:A:H61	27:A:637:A:H5''	1.55	0.72
27:A:271:G:O2'	27:A:272:A:OP2	2.08	0.71
27:A:1534:U:O2'	27:A:1537:G:O6	2.05	0.71
1:a:1028:C:N4	1:a:1029:U:O4	2.22	0.71
5:e:163:GLU:O	8:h:114:ARG:NH2	2.19	0.71
33:G:104:ASN:ND2	33:G:114:ASP:OD1	2.24	0.70
32:F:135:GLN:HG2	32:F:141:ILE:HD13	1.74	0.70
32:F:101:GLU:O	32:F:105:THR:OG1	2.07	0.70
2:b:8:ASP:OD1	2:b:9:MET:N	2.24	0.70
2:b:115:LYS:NZ	2:b:152:LYS:O	2.19	0.70
27:A:1047:G:O2'	27:A:1111:A:N6	2.25	0.70
26:z:140:MET:HE2	26:z:140:MET:HA	1.74	0.69
27:A:1084:A:HO2'	27:A:1085:A:P	2.13	0.69
35:J:109:ILE:O	35:J:113:LYS:N	2.26	0.69
11:k:57:LYS:NZ	64:k:201:HOH:O	2.25	0.69
1:a:1001:C:N4	1:a:1002:G:O6	2.26	0.68
27:A:1060:U:O2'	27:A:1061:U:OP2	2.12	0.68
27:A:2130:U:O2'	27:A:2159:G:N2	2.25	0.68
1:a:677:U:H3	1:a:713:G:H22	1.40	0.68
10:j:52:LEU:HD12	10:j:62:ARG:HD3	1.76	0.68
27:A:276:U:O2	27:A:277:G:N2	2.28	0.67
28:B:5:U:OP1	28:B:61:G:O2'	2.10	0.67
37:M:17:ARG:NE	37:M:47:ILE:HD11	2.09	0.67
1:a:413:G:O2'	1:a:428:G:N2	2.26	0.67
1:a:673:A:H2'	1:a:674:G:C8	2.29	0.67
17:q:47:HIS:NE2	17:q:49:GLU:OE1	2.28	0.67
13:m:11:ASP:HA	13:m:45:ILE:HD11	1.76	0.67
32:F:19:GLU:OE1	32:F:19:GLU:N	2.28	0.67
13:m:54:ASP:OD1	13:m:57:ARG:NH1	2.28	0.66
1:a:662:U:OP1	6:f:93:LYS:NZ	2.24	0.66
32:F:22:TYR:OH	32:F:165:GLU:OE1	2.12	0.66
27:A:2144:G:N2	27:A:2146:C:O2'	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2489:U:O2'	27:A:2490:G:OP1	2.14	0.66
2:b:5:SER:OG	2:b:7:ARG:NH2	2.29	0.65
1:a:22:G:N7	64:a:3207:HOH:O	2.29	0.65
9:i:19:VAL:HG11	9:i:82:GLY:C	2.22	0.65
27:A:1064:C:OP1	35:J:89:GLY:N	2.28	0.64
27:A:1068:G:H21	27:A:1096:A:H5'	1.62	0.64
27:A:2811:G:H1	27:A:2889:C:H5	1.44	0.64
27:A:1250:G:N7	38:N:18:ARG:NH2	2.46	0.64
1:a:1233:G:OP1	9:i:119:ARG:NH1	2.30	0.64
34:H:1:MET:HE1	50:Z:60:ASP:HB3	1.79	0.64
43:S:97:ASP:OD2	44:T:13:ARG:NE	2.31	0.64
4:d:28:ILE:HD13	4:d:34:ILE:HD13	1.80	0.64
27:A:635:C:O2'	27:A:639:U:OP1	2.16	0.63
27:A:84:A:N1	27:A:98:G:O2'	2.29	0.63
27:A:1064:C:O2'	27:A:1065:U:O4'	2.16	0.63
1:a:1530:G:N7	21:u:46:LYS:NZ	2.47	0.63
28:B:119:A:O2'	28:B:120:U:O5'	2.12	0.63
1:a:187:G:N2	1:a:190:A:OP2	2.29	0.62
1:a:823:C:HO2'	8:h:2:SER:N	1.97	0.62
9:i:39:PHE:O	9:i:45:ARG:NE	2.32	0.62
31:E:46:GLN:O	31:E:88:ARG:NH2	2.32	0.62
47:W:18:ASP:OD1	47:W:39:ILE:O	2.16	0.62
27:A:1460:U:O2'	27:A:1461:C:OP1	2.18	0.62
36:L:125:TYR:OH	36:L:132:HIS:NE2	2.32	0.62
4:d:174:ASP:OD1	4:d:176:GLY:N	2.32	0.62
27:A:2150:C:H2'	27:A:2151:U:O4'	1.99	0.62
32:F:17:MET:HE1	32:F:25:VAL:HG23	1.82	0.62
27:A:2453:A:H4'	27:A:2573:C:OP2	2.00	0.62
27:A:1417:C:O2'	27:A:1587:G:O2'	2.17	0.61
10:j:66:GLU:HB2	14:n:99:ALA:HB2	1.82	0.61
27:A:1527:G:N1	27:A:1544:A:OP2	2.32	0.61
27:A:2189:U:O2'	27:A:2190:G:O5'	2.17	0.61
27:A:2758:A:O2'	33:G:38:ASN:ND2	2.33	0.61
3:c:58:GLU:OE1	3:c:65:ARG:NH2	2.33	0.61
27:A:282:A:N6	27:A:359:G:O6	2.33	0.61
11:k:115:PRO:O	11:k:116:ILE:HD13	2.01	0.61
26:z:323:PHE:CE2	26:z:351:VAL:HG11	2.36	0.60
1:a:97:G:O2'	1:a:98:A:OP2	2.19	0.60
1:a:1151:A:H5''	10:j:44:THR:HG23	1.83	0.60
23:w:18:G:HO2'	23:w:57:G:H22	1.43	0.60
27:A:147:C:O2'	27:A:148:U:OP2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:586:A:H5'	31:E:84:THR:HG21	1.84	0.60
37:M:63:VAL:HG12	37:M:107:LEU:HD11	1.83	0.60
51:1:32:ALA:HB2	51:1:37:LEU:HD23	1.83	0.60
27:A:1607:C:N4	27:A:1622:G:OP2	2.26	0.59
1:a:259:G:OP1	20:t:36:TYR:OH	2.19	0.59
1:a:1492:A:O2'	1:a:1493:A:OP2	2.20	0.59
27:A:2291:U:H2'	27:A:2292:U:C6	2.36	0.59
9:i:55:VAL:HG21	9:i:94:LEU:HD13	1.83	0.59
27:A:1062:G:H1'	27:A:1063:G:C8	2.37	0.59
1:a:1448:C:O2'	1:a:1449:C:O5'	2.20	0.59
27:A:568:U:H1'	27:A:2030:6MZ:H9C1	1.84	0.59
42:R:88:ARG:NH2	42:R:110:ILE:O	2.35	0.59
1:a:982:U:H5''	14:n:6:MET:HE2	1.83	0.59
1:a:1005:A:C6	1:a:1024:G:N2	2.70	0.59
1:a:1013:G:N2	1:a:1016:A:OP2	2.28	0.59
23:w:55:PSU:O2'	23:w:57:G:N7	2.29	0.59
4:d:58:LYS:HA	4:d:200:ILE:HD12	1.84	0.59
24:x:58:A:O2'	24:x:60:U:OP2	2.17	0.59
27:A:870:U:OP1	39:O:6:ARG:NE	2.36	0.59
1:a:532:A:N6	1:a:1206:G:O2'	2.33	0.59
20:t:43:ASP:HB3	20:t:46:ALA:HB3	1.85	0.59
27:A:1063:G:H3'	27:A:1064:C:C5'	2.32	0.58
45:U:72:THR:HG21	45:U:108:SER:OG	2.02	0.58
35:J:101:ILE:N	35:J:139:VAL:O	2.35	0.58
9:i:36:GLU:OE1	9:i:36:GLU:N	2.34	0.58
1:a:1055:A:O2'	3:c:161:GLU:OE1	2.20	0.58
27:A:1857:G:H1'	27:A:1885:A:H61	1.68	0.58
27:A:2127:G:O2'	27:A:2128:G:O5'	2.22	0.58
33:G:24:ILE:HD12	33:G:24:ILE:N	2.19	0.58
1:a:251:G:N7	64:a:3212:HOH:O	2.32	0.58
27:A:61:C:OP2	51:1:47:ARG:NH2	2.24	0.58
28:B:7:G:C2'	28:B:8:C:H5'	2.34	0.58
31:E:16:GLU:OE2	31:E:16:GLU:C	2.47	0.58
9:i:21:ILE:HD12	9:i:86:ALA:HB3	1.86	0.58
1:a:1030:U:OP2	1:a:1033:G:N2	2.37	0.57
2:b:15:HIS:HB3	2:b:43:LEU:HD13	1.85	0.57
19:s:9:PRO:HB2	19:s:39:THR:HG21	1.86	0.57
27:A:1417:C:HO2'	27:A:1587:G:HO2'	1.52	0.57
2:b:147:SER:HB3	2:b:148:LEU:HD12	1.87	0.57
27:A:1110:G:HO2'	27:A:1111:A:H8	1.52	0.57
26:z:320:HIS:CD2	26:z:321:THR:HG23	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:T:28:ALA:HB3	44:T:31:GLU:OE1	2.05	0.57
27:A:2547:A:H2'	27:A:2548:U:C6	2.40	0.57
32:F:136:ILE:HA	32:F:141:ILE:HD11	1.86	0.57
1:a:17:U:H2'	1:a:18:C:C6	2.40	0.57
1:a:1189:U:OP1	14:n:98:LYS:NZ	2.37	0.57
1:a:769:G:H4'	1:a:1513:A:H4'	1.84	0.57
1:a:1086:U:H3	1:a:1099:G:H22	1.53	0.57
1:a:1317:C:O2	19:s:37:ARG:NH2	2.37	0.57
7:g:69:VAL:HG21	7:g:104:ILE:HD11	1.87	0.57
51:l:14:LEU:HD11	51:l:60:LYS:HZ2	1.70	0.57
1:a:673:A:HO2'	1:a:674:G:P	2.26	0.56
27:A:78:U:OP1	51:l:7:ARG:NH2	2.33	0.56
11:k:114:THR:HG21	21:u:32:VAL:HG21	1.86	0.56
27:A:1338:G:O2'	27:A:1393:A:N1	2.34	0.56
27:A:1065:U:O2	27:A:1074:G:N2	2.39	0.56
32:F:107:ALA:HB1	32:F:137:ILE:HD12	1.87	0.56
26:z:141:VAL:HG11	26:z:147:LEU:HD13	1.86	0.56
27:A:1187:G:H5''	44:T:83:TYR:CE1	2.41	0.56
29:C:29:PRO:HG2	29:C:34:LEU:HD11	1.87	0.56
1:a:1373:G:OP2	9:i:73:SER:OG	2.23	0.56
2:b:30:PHE:HE1	2:b:49:MET:HE1	1.70	0.56
27:A:138:U:O2'	27:A:141:G:O6	2.24	0.56
27:A:593:U:H2'	27:A:594:U:C6	2.41	0.56
27:A:1904:G:O2'	27:A:1928:A:N1	2.39	0.56
28:B:50:A:O2'	28:B:51:G:O5'	2.23	0.56
54:4:43:ILE:HG22	54:4:49:TYR:HB2	1.86	0.56
2:b:30:PHE:CE1	2:b:49:MET:HE1	2.41	0.56
27:A:2064:C:H2'	27:A:2065:C:C6	2.41	0.56
31:E:12:LEU:HD12	31:E:13:THR:N	2.22	0.55
15:o:78:TYR:OH	15:o:89:ARG:O	2.19	0.55
26:z:310:TYR:OH	26:z:316:GLU:OE2	2.25	0.55
27:A:145:C:O2'	27:A:146:A:OP2	2.20	0.55
27:A:1585:C:H2'	27:A:1586:A:O4'	2.07	0.55
1:a:1027:C:N4	1:a:1035:A:N1	2.53	0.55
27:A:2111:U:O5'	27:A:2118:U:O2'	2.24	0.55
47:W:98:SER:OG	47:W:98:SER:O	2.20	0.55
27:A:2154:A:H2'	27:A:2155:U:O4'	2.06	0.55
27:A:2328:A:H2'	27:A:2329:U:C6	2.42	0.55
27:A:210:C:OP1	56:6:29:GLN:NE2	2.35	0.55
27:A:856:G:H2'	27:A:857:G:C8	2.41	0.55
27:A:2784:U:H2'	27:A:2785:C:H5''	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:3:C:O2'	28:B:4:C:P	2.65	0.55
1:a:404:G:N7	4:d:2:ALA:HB3	2.21	0.54
11:k:94:GLU:OE2	21:u:20:LYS:HD3	2.07	0.54
27:A:548:G:H2'	27:A:549:G:N9	2.21	0.54
27:A:642:U:O2'	27:A:644:A:N7	2.36	0.54
27:A:1856:U:H2'	27:A:1857:G:O4'	2.07	0.54
27:A:2591:C:H2'	27:A:2592:G:C8	2.42	0.54
26:z:149:LEU:O	26:z:153:GLU:HG3	2.07	0.54
27:A:1003:G:O2'	27:A:1010:A:N1	2.37	0.54
3:c:53:SER:OG	3:c:112:ASP:OD2	2.19	0.54
27:A:142:A:O2'	27:A:143:C:P	2.66	0.54
1:a:131:A:O2'	1:a:262:A:N3	2.33	0.54
2:b:72:THR:HG22	2:b:94:HIS:O	2.06	0.54
6:f:27:ALA:O	6:f:31:GLY:N	2.36	0.54
27:A:849:A:H2'	27:A:850:U:C6	2.42	0.54
27:A:1668:A:O2'	27:A:1674:G:N7	2.37	0.54
27:A:1802:A:H2'	27:A:1803:A:C8	2.43	0.54
1:a:96:U:O2'	1:a:97:G:P	2.65	0.54
6:f:39:LEU:HD22	6:f:62:MET:HG2	1.90	0.54
13:m:45:ILE:C	13:m:45:ILE:HD12	2.32	0.54
27:A:2128:G:H21	27:A:2173:A:C4'	2.19	0.54
11:k:85:MET:HE1	18:r:73:ARG:HH12	1.72	0.54
27:A:1141:U:H4'	27:A:1142:A:O4'	2.08	0.54
9:i:32:GLN:OE1	9:i:32:GLN:HA	2.08	0.54
27:A:811:U:H2'	38:N:21:ARG:HA	1.90	0.54
1:a:1486:G:H2'	1:a:1487:G:O4'	2.07	0.53
27:A:2627:G:O2'	27:A:2781:A:N1	2.39	0.53
3:c:11:ARG:NH2	3:c:175:LEU:O	2.40	0.53
27:A:64:A:H2'	27:A:65:U:C6	2.42	0.53
2:b:67:ILE:N	2:b:89:GLN:OE1	2.41	0.53
26:z:337:ASP:OD1	26:z:337:ASP:N	2.41	0.53
27:A:1778:U:H2'	27:A:1784:A:N6	2.23	0.53
44:T:14:VAL:HG11	44:T:20:VAL:HG21	1.91	0.53
1:a:520:A:O2'	12:l:70:GLU:OE1	2.22	0.53
4:d:201:VAL:O	4:d:205:SER:OG	2.22	0.53
11:k:97:ILE:HG22	21:u:12:PHE:HZ	1.74	0.53
27:A:2291:U:OP1	27:A:2380:C:O2'	2.20	0.53
1:a:147:G:H2'	1:a:148:G:C8	2.44	0.53
1:a:195:A:O2'	1:a:196:A:O5'	2.27	0.53
10:j:84:VAL:HG13	10:j:88:MET:HE2	1.91	0.53
27:A:528:A:C2	27:A:2043:C:H4'	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:995:C:O2	36:L:3:THR:HG22	2.09	0.53
27:A:1939:5MU:OP1	27:A:2604:PSU:O2'	2.27	0.53
1:a:1218:C:H2'	1:a:1219:A:C8	2.44	0.53
27:A:639:U:H2'	27:A:640:C:C6	2.44	0.53
3:c:35:SER:OG	3:c:59:ARG:NH2	2.42	0.53
27:A:1942:C:OP2	27:A:1943:U:O2'	2.25	0.53
7:g:129:GLU:OE2	7:g:129:GLU:O	2.27	0.53
27:A:1469:A:H2'	27:A:1470:A:C8	2.44	0.53
27:A:2129:C:H42	27:A:2160:C:H42	1.56	0.53
27:A:784:G:H5'	27:A:785:G:OP1	2.09	0.52
27:A:2129:C:N4	27:A:2160:C:H42	2.06	0.52
1:a:189:A:H2'	1:a:190:A:O4'	2.09	0.52
1:a:922:G:H2'	1:a:923:A:C8	2.44	0.52
27:A:1094:U:N3	27:A:1097:U:OP2	2.34	0.52
27:A:2144:G:C2	27:A:2146:C:H1'	2.45	0.52
27:A:2590:A:N3	64:A:3818:HOH:O	2.34	0.52
37:M:47:ILE:HG23	37:M:48:PRO:HD2	1.92	0.52
53:3:20:ASN:ND2	53:3:22:MET:HE2	2.25	0.52
27:A:1980:G:O2'	27:A:1982:U:OP2	2.27	0.52
27:A:144:A:O2'	27:A:145:C:H5'	2.09	0.52
29:C:165:VAL:HG21	29:C:181:MET:HE1	1.90	0.52
32:F:137:ILE:HD11	32:F:138:PHE:CE2	2.44	0.52
39:O:127:LYS:HD3	39:O:128:THR:N	2.24	0.52
1:a:83:C:O2'	1:a:87:C:N4	2.42	0.52
7:g:70:ARG:NH1	7:g:97:ASN:OD1	2.38	0.52
27:A:528:A:OP2	27:A:528:A:C8	2.63	0.52
27:A:1028:A:N6	27:A:1125:G:H2'	2.25	0.52
26:z:186:GLU:O	26:z:190:LEU:HD23	2.10	0.52
32:F:102:ARG:NH1	53:3:9:TYR:OH	2.42	0.52
1:a:411:A:C4	1:a:413:G:H1'	2.45	0.52
1:a:1005:A:N6	1:a:1024:G:H21	2.06	0.52
1:a:414:A:O2'	1:a:415:A:OP1	2.27	0.52
23:w:21:A:H61	23:w:46:G7M:H2'	1.74	0.52
1:a:502:A:H2'	1:a:503:C:O4'	2.10	0.52
26:z:67:HIS:O	62:z:402:MQH:N24	2.43	0.52
29:C:107:PRO:HD2	29:C:110:LEU:HD22	1.92	0.52
1:a:1038:C:N4	1:a:1039:G:O6	2.43	0.52
27:A:353:C:C2	27:A:354:A:C8	2.98	0.52
27:A:1790:C:H2'	27:A:1791:A:C5	2.45	0.52
37:M:17:ARG:HE	37:M:47:ILE:HD11	1.74	0.52
6:f:26:THR:HG23	6:f:36:ILE:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:548:G:H2'	27:A:549:G:C1'	2.40	0.51
1:a:264:C:H2'	1:a:265:G:O4'	2.09	0.51
1:a:1391:U:H2'	1:a:1392:G:C8	2.45	0.51
26:z:259:VAL:O	26:z:265:LEU:O	2.28	0.51
27:A:594:U:H2'	27:A:595:C:C6	2.45	0.51
27:A:2143:C:N4	27:A:2144:G:O6	2.43	0.51
47:W:97:LYS:O	47:W:98:SER:OG	2.27	0.51
1:a:714:G:H2'	1:a:715:A:C8	2.45	0.51
27:A:1664:A:N3	37:M:67:LYS:NZ	2.59	0.51
27:A:1932:A:H2'	27:A:1933:G:O4'	2.10	0.51
27:A:2303:G:O2'	27:A:2304:G:P	2.69	0.51
1:a:1492:A:H5''	12:l:44:LYS:HG3	1.93	0.51
4:d:188:ARG:NE	4:d:197:GLU:OE2	2.41	0.51
27:A:279:A:H61	27:A:362:A:C4'	2.23	0.51
2:b:68:LEU:HD23	2:b:161:LEU:CD1	2.41	0.51
27:A:2189:U:HO2'	27:A:2190:G:C5'	2.23	0.51
27:A:2302:U:C2'	27:A:2303:G:H5'	2.40	0.51
1:a:384:G:H2'	1:a:385:C:C6	2.45	0.51
1:a:1530:G:H2'	1:a:1531:A:C8	2.46	0.51
7:g:129:GLU:OE2	7:g:131:LYS:HG2	2.10	0.51
1:a:747:A:H2'	1:a:748:G:O4'	2.11	0.51
1:a:1273:C:H2'	1:a:1274:A:O4'	2.11	0.51
1:a:1427:C:H2'	1:a:1428:A:H5''	1.93	0.51
4:d:99:ASP:OD1	4:d:100:ASN:N	2.44	0.51
11:k:97:ILE:HG22	21:u:12:PHE:CZ	2.46	0.51
24:x:45:U:O2'	24:x:46:G7M:OP1	2.28	0.51
27:A:2327:A:H2'	27:A:2328:A:C8	2.46	0.51
28:B:9:G:O2'	28:B:10:G:P	2.68	0.51
1:a:946:A:H2'	1:a:947:G:C8	2.46	0.51
1:a:1098:C:O2'	21:u:71:TYR:O	2.29	0.51
2:b:27:MET:HE2	2:b:188:ASP:O	2.10	0.51
13:m:50:GLU:HA	13:m:50:GLU:OE1	2.11	0.51
27:A:391:A:O2'	27:A:410:G:OP1	2.25	0.51
1:a:662:U:O2'	1:a:836:G:OP1	2.27	0.51
10:j:22:THR:HG21	10:j:39:PRO:HB3	1.91	0.51
27:A:581:C:H2'	27:A:582:A:C8	2.46	0.51
1:a:694:A:H2'	1:a:695:A:O4'	2.11	0.50
14:n:49:GLN:HE22	19:s:12:ASP:HA	1.75	0.50
27:A:2138:G:C6	27:A:2154:A:N1	2.79	0.50
34:H:6:LEU:HD11	34:H:37:VAL:HG13	1.93	0.50
1:a:107:G:O6	20:t:10:ARG:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:429:U:O2'	4:d:31:LYS:NZ	2.41	0.50
1:a:1225:A:H2'	1:a:1226:C:C5	2.46	0.50
2:b:135:LEU:C	2:b:135:LEU:HD13	2.37	0.50
3:c:50:ALA:O	3:c:70:THR:OG1	2.27	0.50
27:A:1149:G:H2'	27:A:1150:C:C6	2.46	0.50
42:R:100:LEU:HD11	42:R:110:ILE:HD11	1.93	0.50
1:a:522:C:H41	12:l:50:ARG:NH2	2.10	0.50
27:A:144:A:O2'	27:A:145:C:H6	1.93	0.50
27:A:833:A:H2'	27:A:834:G:C8	2.47	0.50
1:a:264:C:O2'	17:q:66:PRO:O	2.27	0.50
1:a:413:G:HO2'	1:a:428:G:N2	2.08	0.50
26:z:166:ASP:OD1	26:z:166:ASP:N	2.45	0.50
27:A:2071:A:H2'	27:A:2072:C:C6	2.46	0.50
28:B:114:C:O2'	28:B:115:A:O5'	2.28	0.50
27:A:2065:C:H4'	27:A:2251:OMG:HM22	1.93	0.50
1:a:695:A:H2'	1:a:696:A:C8	2.46	0.50
4:d:9:LEU:HD13	4:d:32:CYS:HB3	1.94	0.50
27:A:2757:A:O2'	27:A:2758:A:O5'	2.26	0.50
31:E:16:GLU:OE2	31:E:16:GLU:O	2.29	0.50
6:f:10:VAL:HG23	6:f:83:ALA:C	2.36	0.50
26:z:163:PHE:O	26:z:165:GLY:N	2.44	0.50
27:A:1857:G:H1'	27:A:1885:A:N6	2.27	0.50
33:G:35:ARG:HG3	33:G:36:THR:N	2.25	0.50
1:a:97:G:O2'	1:a:98:A:P	2.70	0.50
4:d:101:VAL:O	4:d:105:MET:HG3	2.12	0.50
18:r:71:THR:OG1	18:r:73:ARG:O	2.26	0.50
54:4:36:GLU:OE1	54:4:46:ASP:OD1	2.29	0.50
1:a:8:A:N6	4:d:202:GLU:O	2.44	0.50
47:W:49:VAL:HG23	47:W:52:LEU:O	2.11	0.50
1:a:1315:U:H2'	1:a:1316:G:O4'	2.12	0.49
1:a:1317:C:OP2	14:n:28:LYS:HE2	2.12	0.49
1:a:1416:G:N7	64:a:3216:HOH:O	2.34	0.49
3:c:56:VAL:HB	3:c:67:THR:HG23	1.93	0.49
27:A:554:U:H2'	27:A:555:G:O4'	2.12	0.49
27:A:1434:A:H2'	27:A:1435:G:C8	2.46	0.49
27:A:2788:C:H2'	27:A:2789:C:C6	2.47	0.49
28:B:9:G:HO2'	28:B:10:G:P	2.34	0.49
39:O:25:ASP:O	39:O:66:ARG:NH1	2.44	0.49
27:A:2178:C:H2'	27:A:2179:C:H5'	1.94	0.49
31:E:1:MET:HE1	31:E:19:PHE:O	2.12	0.49
33:G:73:ASN:O	33:G:77:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:31:G:O2'	1:a:48:C:N4	2.44	0.49
1:a:728:A:H2'	1:a:729:A:C8	2.48	0.49
26:z:121:LEU:O	26:z:125:GLN:HG2	2.12	0.49
27:A:58:G:O2'	27:A:73:A:N1	2.44	0.49
55:5:28:ARG:H	55:5:28:ARG:HE	1.59	0.49
1:a:67:C:HO2'	1:a:171:A:HO2'	1.61	0.49
4:d:96:GLY:O	4:d:137:VAL:HG13	2.12	0.49
27:A:1370:C:H2'	27:A:1371:G:O4'	2.12	0.49
27:A:2489:U:O2'	27:A:2490:G:H5'	2.12	0.49
1:a:600:A:OP2	8:h:88:ARG:HD2	2.13	0.49
27:A:1079:C:H41	27:A:1088:A:P	2.35	0.49
27:A:2191:A:O2'	27:A:2192:U:P	2.69	0.49
38:N:57:LEU:HD22	57:7:54:ASP:HB3	1.95	0.49
47:W:94:ARG:HB3	47:W:103:ILE:HD12	1.94	0.49
24:x:23:A:H2'	24:x:24:G:C8	2.47	0.49
26:z:342:ILE:HG23	26:z:359:MET:HE2	1.95	0.49
41:Q:39:VAL:HG11	41:Q:87:ILE:HD13	1.95	0.49
1:a:999:C:N3	1:a:1042:A:N6	2.60	0.49
9:i:7:TYR:HH	9:i:9:THR:HG1	1.60	0.49
27:A:460:A:H2'	27:A:461:C:O4'	2.13	0.49
27:A:1433:A:H2'	27:A:1434:A:O4'	2.12	0.49
1:a:945:G:C2	1:a:946:A:C8	3.01	0.49
1:a:1062:U:H2'	1:a:1063:C:C6	2.47	0.49
25:y:104:LYS:HE2	27:A:2451:A:N1	2.28	0.49
28:B:51:G:H2'	28:B:52:A:C8	2.47	0.49
46:V:4:GLU:HG3	46:V:49:LYS:CE	2.43	0.49
27:A:813:U:H2'	27:A:814:C:C6	2.48	0.49
27:A:857:G:H2'	27:A:858:G:O4'	2.13	0.49
28:B:50:A:O2'	28:B:51:G:P	2.71	0.49
30:D:25:THR:HG21	30:D:193:VAL:HG13	1.94	0.48
31:E:153:LEU:HD12	31:E:169:VAL:HG12	1.95	0.48
40:P:86:ARG:NH2	40:P:117:ASP:OD1	2.42	0.48
10:j:77:VAL:O	10:j:78:GLU:HG3	2.13	0.48
27:A:1361:G:H2'	27:A:1362:C:C6	2.48	0.48
27:A:1541:C:O2'	27:A:1542:U:H5'	2.13	0.48
27:A:1794:A:H2'	27:A:1795:C:C6	2.48	0.48
27:A:2312:U:O2'	27:A:2313:C:P	2.71	0.48
40:P:30:ARG:NH1	40:P:74:GLU:OE2	2.45	0.48
17:q:19:LYS:HA	17:q:48:ASP:O	2.13	0.48
27:A:145:C:O2'	27:A:146:A:P	2.72	0.48
27:A:468:G:N7	56:6:39:ARG:NH2	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:933:A:H5'	27:A:934:U:OP2	2.14	0.48
1:a:401:C:O2'	1:a:621:A:N3	2.43	0.48
10:j:7:ARG:HD3	10:j:73:LEU:HD11	1.95	0.48
17:q:54:GLY:N	17:q:57:ASP:OD2	2.46	0.48
19:s:13:LEU:HD11	19:s:17:LYS:NZ	2.28	0.48
27:A:706:A:OP1	29:C:7:LYS:NZ	2.46	0.48
27:A:2461:A:H2'	27:A:2462:C:C6	2.49	0.48
52:2:11:ARG:HG2	52:2:11:ARG:HH11	1.78	0.48
27:A:282:A:H2'	27:A:283:G:O4'	2.14	0.48
27:A:1084:A:H1'	27:A:1105:U:O2'	2.13	0.48
27:A:1266:G:O2'	27:A:2012:G:O6	2.27	0.48
1:a:320:A:H2'	1:a:321:A:O4'	2.13	0.48
27:A:839:U:H2'	27:A:840:C:C6	2.48	0.48
36:L:3:THR:HG21	43:S:61:TRP:HE1	1.77	0.48
23:w:26:A:N1	23:w:44:G:C6	2.82	0.48
27:A:265:A:N1	27:A:427:U:O2'	2.46	0.48
27:A:644:A:H2'	27:A:645:C:O4'	2.14	0.48
28:B:50:A:HO2'	28:B:51:G:C5'	2.25	0.48
27:A:1418:G:O2'	27:A:1419:A:H5''	2.14	0.48
1:a:382:A:H2'	1:a:383:A:C8	2.48	0.48
26:z:152:MET:O	26:z:156:GLU:HG2	2.14	0.48
27:A:120:U:H5''	27:A:122:G:OP2	2.13	0.48
27:A:1327:A:H2'	27:A:1328:A:O4'	2.13	0.48
1:a:51:A:N7	1:a:114:U:O2'	2.46	0.48
1:a:131:A:H2'	1:a:132:C:C6	2.49	0.48
26:z:319:ARG:NH2	26:z:322:PRO:O	2.40	0.48
27:A:1:G:H2'	27:A:2:G:C8	2.49	0.48
27:A:352:A:H2'	27:A:353:C:O4'	2.14	0.48
27:A:1542:U:H2'	27:A:1543:G:O4'	2.14	0.48
27:A:2709:G:OP1	40:P:18:GLN:NE2	2.46	0.48
27:A:2785:C:H5''	27:A:2785:C:H6	1.79	0.48
1:a:206:C:H2'	1:a:207:C:C6	2.49	0.47
1:a:524:G:H2'	1:a:525:C:C6	2.49	0.47
2:b:148:LEU:HD23	2:b:151:ILE:HD11	1.96	0.47
19:s:42:PRO:O	19:s:45:ILE:HG12	2.14	0.47
27:A:914:G:H5'	27:A:915:C:OP2	2.14	0.47
27:A:2139:U:H2'	27:A:2140:G:O4'	2.14	0.47
28:B:66:A:H4'	28:B:67:G:OP1	2.13	0.47
29:C:31:ALA:HA	29:C:34:LEU:HD12	1.96	0.47
2:b:7:ARG:H	2:b:7:ARG:HE	1.62	0.47
2:b:125:THR:O	2:b:127:GLU:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:115:PRO:C	11:k:116:ILE:HD13	2.38	0.47
27:A:2038:G:H2'	27:A:2039:U:O4'	2.14	0.47
26:z:8:ARG:CZ	26:z:266:LEU:HD22	2.44	0.47
27:A:1027:A:C2	27:A:2488:G:H5'	2.49	0.47
27:A:1064:C:N4	27:A:1076:C:C5	2.82	0.47
27:A:2149:U:C2	27:A:2150:C:C5	3.02	0.47
27:A:2189:U:H2'	27:A:2190:G:H8	1.79	0.47
29:C:91:ILE:HD12	29:C:103:TYR:CD1	2.49	0.47
5:e:107:ALA:HB2	5:e:125:ALA:HB3	1.96	0.47
27:A:528:A:C2	27:A:2042:A:H2'	2.50	0.47
27:A:1577:C:H2'	27:A:1578:U:O4'	2.15	0.47
27:A:2115:G:O2'	27:A:2117:A:N6	2.47	0.47
31:E:1:MET:N	31:E:14:VAL:O	2.45	0.47
1:a:579:A:H2'	1:a:580:C:C6	2.49	0.47
1:a:1103:C:OP1	2:b:95:ARG:NH2	2.45	0.47
10:j:21:ALA:HB1	10:j:92:LEU:HD13	1.95	0.47
23:w:26:A:N1	23:w:44:G:O6	2.48	0.47
26:z:265:LEU:O	26:z:266:LEU:HB2	2.14	0.47
27:A:1001:A:H2'	27:A:1002:G:O4'	2.14	0.47
53:3:9:TYR:HD1	53:3:27:THR:HG23	1.80	0.47
53:3:35:ASP:OD1	53:3:35:ASP:N	2.47	0.47
1:a:69:G:H2'	1:a:70:U:C6	2.48	0.47
1:a:1005:A:H62	1:a:1024:G:N2	2.12	0.47
14:n:36:ALA:O	14:n:41:ARG:NH2	2.47	0.47
27:A:1037:G:H2'	27:A:1038:G:H5''	1.97	0.47
27:A:1128:G:C8	27:A:2490:G:OP1	2.68	0.47
27:A:2331:G:O2'	27:A:2336:A:N1	2.31	0.47
38:N:81:ASP:HA	38:N:84:LYS:HD2	1.96	0.47
39:O:60:GLN:OE1	39:O:60:GLN:HA	2.14	0.47
48:X:48:MET:HE2	48:X:84:PRO:O	2.14	0.47
1:a:371:A:H2'	1:a:372:C:O4'	2.15	0.47
2:b:78:GLU:CD	2:b:78:GLU:H	2.23	0.47
26:z:382:ARG:HB3	26:z:382:ARG:CZ	2.45	0.47
26:z:393:LEU:C	26:z:393:LEU:HD13	2.40	0.47
27:A:144:A:HO2'	27:A:145:C:H6	1.63	0.47
27:A:493:G:H2'	27:A:494:G:O4'	2.15	0.47
27:A:2895:G:H2'	27:A:2896:C:C6	2.50	0.47
28:B:114:C:O2'	28:B:115:A:P	2.72	0.47
53:3:37:CYS:SG	53:3:40:CYS:HB2	2.54	0.47
57:7:14:PHE:C	57:7:15:LYS:HD2	2.39	0.47
1:a:555:U:H2'	1:a:556:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:986:U:H2'	1:a:987:G:O4'	2.14	0.47
1:a:1356:G:H2'	1:a:1357:A:C8	2.50	0.47
2:b:138:THR:O	2:b:142:GLU:HG3	2.15	0.47
27:A:1405:U:H2'	27:A:1406:U:C6	2.50	0.47
27:A:2128:G:H2'	27:A:2129:C:C6	2.50	0.47
27:A:2850:A:N7	27:A:2868:A:O2'	2.38	0.47
1:a:337:G:H2'	1:a:338:A:C8	2.50	0.47
1:a:920:U:H2'	1:a:921:U:C6	2.50	0.47
3:c:12:LEU:O	3:c:16:LYS:O	2.33	0.47
27:A:1635:A:OP2	64:A:3802:HOH:O	2.20	0.47
27:A:1848:A:H2'	27:A:1849:G:O4'	2.15	0.47
27:A:2537:U:H2'	27:A:2538:C:C6	2.50	0.47
42:R:27:GLU:OE2	42:R:29:LYS:NZ	2.44	0.47
48:X:43:ASP:OD1	48:X:46:LYS:HG3	2.15	0.47
27:A:1046:A:O2'	27:A:1047:G:OP2	2.30	0.47
27:A:1478:G:H1	27:A:1513:U:H3	1.61	0.47
27:A:2243:U:H2'	27:A:2244:U:C6	2.50	0.47
27:A:2514:U:H2'	27:A:2515:C:C6	2.49	0.47
28:B:50:A:O2'	28:B:51:G:C5'	2.63	0.47
52:2:26:GLY:C	52:2:47:MET:HE1	2.39	0.47
23:w:54:5MU:OP1	26:z:320:HIS:NE2	2.37	0.46
27:A:1386:C:H2'	27:A:1387:A:C8	2.50	0.46
27:A:1505:A:H2'	27:A:1506:U:O4'	2.15	0.46
27:A:1637:A:H5'	27:A:1760:C:O2'	2.15	0.46
27:A:2182:U:H2'	27:A:2183:A:H8	1.80	0.46
27:A:2300:C:H2'	27:A:2301:C:C6	2.50	0.46
27:A:2757:A:HO2'	27:A:2758:A:P	2.38	0.46
27:A:2888:C:H2'	27:A:2889:C:O2	2.15	0.46
32:F:163:ASP:N	32:F:163:ASP:OD1	2.47	0.46
1:a:757:U:OP1	1:a:822:U:O2'	2.30	0.46
1:a:1314:C:H2'	1:a:1315:U:C6	2.51	0.46
27:A:2506:U:H4'	27:A:2507:C:OP1	2.14	0.46
28:B:106:G:H2'	28:B:107:G:O4'	2.15	0.46
34:H:29:PHE:O	34:H:32:PRO:HD2	2.15	0.46
39:O:78:LEU:HD23	39:O:79:ALA:N	2.29	0.46
51:1:14:LEU:HD11	51:1:60:LYS:NZ	2.28	0.46
1:a:212:G:C4	1:a:213:G:C8	3.04	0.46
1:a:594:U:H2'	1:a:595:A:O4'	2.14	0.46
1:a:1074:G:O2'	1:a:1101:A:N1	2.44	0.46
27:A:2189:U:O2'	27:A:2190:G:P	2.73	0.46
1:a:1170:A:H2'	1:a:1171:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:8:ILE:HD12	10:j:76:ILE:CD1	2.46	0.46
23:w:26:A:C2	23:w:27:C:C6	3.03	0.46
26:z:187:ALA:O	26:z:191:GLU:OE1	2.34	0.46
27:A:2025:C:H2'	27:A:2026:U:C6	2.50	0.46
1:a:19:A:O2'	1:a:572:A:N1	2.46	0.46
9:i:21:ILE:HD12	9:i:86:ALA:CB	2.45	0.46
27:A:476:G:H4'	27:A:502:A:N1	2.31	0.46
27:A:1570:A:H2'	27:A:1571:A:C8	2.51	0.46
27:A:2273:A:H2'	27:A:2274:A:C8	2.51	0.46
57:7:31:HIS:CG	57:7:32:ILE:HG13	2.51	0.46
1:a:1071:C:H2'	1:a:1072:G:H8	1.80	0.46
1:a:1130:A:C8	1:a:1146:A:N1	2.84	0.46
6:f:9:MET:HE3	6:f:86:ARG:HB3	1.97	0.46
10:j:10:LEU:CD1	10:j:98:VAL:HG13	2.46	0.46
10:j:77:VAL:HG22	10:j:78:GLU:H	1.81	0.46
27:A:12:U:O2'	27:A:13:A:P	2.73	0.46
27:A:1039:A:H2	27:A:1116:G:H22	1.63	0.46
27:A:1824:G:O3'	29:C:247:PRO:HD3	2.16	0.46
27:A:2191:A:HO2'	27:A:2192:U:P	2.38	0.46
41:Q:52:SER:OG	41:Q:54:VAL:HG22	2.16	0.46
1:a:523:A:C2	12:l:88:LYS:HB3	2.51	0.46
9:i:55:VAL:HG23	9:i:94:LEU:HD22	1.97	0.46
27:A:1180:U:O2'	27:A:1181:U:H5'	2.16	0.46
27:A:2074:U:H2'	27:A:2075:U:C6	2.50	0.46
27:A:2186:G:H2'	27:A:2187:U:O4'	2.16	0.46
30:D:156:PHE:CE1	36:L:81:ILE:HD13	2.51	0.46
1:a:1036:A:H2'	1:a:1037:C:C4'	2.46	0.46
26:z:155:ARG:NH1	26:z:165:GLY:O	2.42	0.46
27:A:468:G:H5''	31:E:55:SER:HB3	1.98	0.46
27:A:1197:G:H2'	27:A:1198:U:H6	1.81	0.46
27:A:1874:C:H2'	27:A:1875:G:O4'	2.16	0.46
33:G:98:VAL:HG22	33:G:103:ILE:HG12	1.97	0.46
1:a:22:G:O2'	1:a:913:A:N1	2.42	0.46
1:a:839:C:H2'	1:a:839:C:O2	2.16	0.46
1:a:1435:G:H2'	1:a:1436:U:C6	2.50	0.46
2:b:6:MET:O	2:b:10:LEU:HD23	2.15	0.46
15:o:25:THR:HG21	15:o:70:LEU:HB2	1.98	0.46
27:A:284:U:H2'	27:A:285:G:H8	1.79	0.46
27:A:742:A:H2'	27:A:743:A:C8	2.51	0.46
27:A:2127:G:O2'	27:A:2128:G:O4'	2.31	0.46
27:A:2303:G:O2'	27:A:2304:G:OP2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:24:VAL:HG12	30:D:178:VAL:HG21	1.97	0.46
45:U:59:GLU:OE2	45:U:66:ILE:CG2	2.64	0.46
27:A:1110:G:O2'	27:A:1111:A:P	2.74	0.46
27:A:2187:U:C2	27:A:2188:U:C5	3.03	0.46
32:F:160:ALA:HB1	32:F:165:GLU:HB3	1.97	0.46
1:a:1323:G:H2'	1:a:1324:A:C8	2.51	0.45
6:f:21:MET:HB2	6:f:25:TYR:CE1	2.52	0.45
7:g:72:THR:HG23	7:g:96:ARG:HH21	1.82	0.45
10:j:8:ILE:HD12	10:j:76:ILE:HD11	1.98	0.45
32:F:163:ASP:O	32:F:167:ARG:N	2.42	0.45
1:a:246:A:C2	1:a:282:A:C5	3.04	0.45
1:a:439:U:H5''	4:d:121:LYS:HD2	1.97	0.45
27:A:586:A:N1	27:A:809:G:O2'	2.41	0.45
27:A:1182:G:H2'	27:A:1183:U:O4'	2.16	0.45
27:A:1198:U:H2'	27:A:1199:U:C6	2.50	0.45
27:A:2131:U:H5'	27:A:2133:G:H4'	1.99	0.45
1:a:330:C:O2	1:a:330:C:O4'	2.33	0.45
1:a:613:C:H2'	1:a:614:C:C6	2.51	0.45
2:b:10:LEU:HD22	2:b:43:LEU:HD22	1.97	0.45
10:j:22:THR:CG2	10:j:39:PRO:HB3	2.47	0.45
27:A:851:C:H2'	27:A:852:U:C6	2.52	0.45
27:A:1297:C:O2'	27:A:1302:A:N1	2.49	0.45
27:A:2455:G:H2'	27:A:2456:C:C6	2.52	0.45
27:A:2810:A:H2'	27:A:2811:G:O4'	2.17	0.45
28:B:11:C:OP1	49:Y:72:LYS:NZ	2.49	0.45
38:N:141:LYS:NZ	38:N:143:GLU:OE1	2.49	0.45
44:T:5:PHE:HB3	44:T:59:ILE:HD12	1.98	0.45
1:a:407:U:O2'	4:d:113:GLU:OE1	2.34	0.45
26:z:125:GLN:HE22	26:z:312:LEU:HD22	1.81	0.45
26:z:218:VAL:HG11	26:z:287:ILE:CG2	2.45	0.45
27:A:1056:G:O2'	27:A:1103:A:N6	2.47	0.45
27:A:1682:G:H2'	27:A:1683:U:C6	2.52	0.45
27:A:1703:G:H2'	27:A:1704:C:C6	2.52	0.45
27:A:1916:A:H2'	27:A:1917:PSU:O4'	2.15	0.45
27:A:2144:G:C6	27:A:2148:G:C6	3.04	0.45
28:B:33:G:O2'	28:B:34:A:H5'	2.17	0.45
46:V:13:ALA:HB1	51:1:33:ALA:HB1	1.99	0.45
1:a:767:A:H2'	1:a:768:A:O4'	2.17	0.45
2:b:196:VAL:HG22	2:b:199:VAL:HG22	1.97	0.45
27:A:1537:G:H2'	27:A:1538:G:O4'	2.16	0.45
27:A:1796:U:H2'	27:A:1797:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:56:LYS:NZ	40:P:90:ARG:O	2.44	0.45
1:a:82:G:H2'	1:a:83:C:O4'	2.16	0.45
1:a:135:C:O2	16:p:1:MET:HB2	2.16	0.45
1:a:213:G:C8	1:a:214:C:C5	3.04	0.45
1:a:1320:C:O2	19:s:36:ARG:NH2	2.46	0.45
27:A:549:G:H2'	27:A:550:C:C6	2.52	0.45
27:A:612:G:O2'	27:A:614:A:N7	2.44	0.45
27:A:1533:C:H2'	27:A:1534:U:O4'	2.16	0.45
27:A:2052:A:H4'	30:D:148:GLN:O	2.16	0.45
27:A:2145:C:H3'	27:A:2146:C:H5'	1.98	0.45
28:B:14:U:OP2	28:B:70:C:O2'	2.29	0.45
30:D:110:THR:HG23	30:D:202:ILE:HB	1.97	0.45
7:g:88:PRO:HG2	7:g:152:ALA:HB2	1.98	0.45
23:w:65:U:H4'	26:z:330:GLN:OE1	2.17	0.45
26:z:218:VAL:HG11	26:z:287:ILE:HG23	1.98	0.45
26:z:393:LEU:HD13	26:z:393:LEU:O	2.17	0.45
27:A:1786:A:H1'	27:A:1938:A:N6	2.31	0.45
28:B:3:C:O2'	28:B:4:C:OP1	2.34	0.45
46:V:24:MET:CE	46:V:30:ILE:HG23	2.47	0.45
1:a:545:C:OP1	4:d:58:LYS:NZ	2.50	0.45
1:a:1023:U:H2'	1:a:1024:G:C8	2.51	0.45
27:A:1060:U:HO2'	27:A:1061:U:P	2.37	0.45
31:E:153:LEU:CD1	31:E:169:VAL:HG12	2.47	0.45
1:a:1428:A:H5''	1:a:1428:A:H8	1.82	0.45
1:a:1518:MA6:H103	1:a:1519:MA6:N6	2.32	0.45
5:e:61:GLN:HG2	5:e:65:GLU:OE2	2.17	0.45
13:m:19:LEU:HB2	13:m:30:SER:OG	2.17	0.45
26:z:348:VAL:O	26:z:348:VAL:HG22	2.17	0.45
27:A:142:A:O2'	27:A:143:C:O5'	2.29	0.45
27:A:634:C:H2'	27:A:635:C:C6	2.51	0.45
27:A:969:G:H2'	27:A:970:U:C6	2.52	0.45
27:A:2176:A:H2'	27:A:2177:C:C6	2.51	0.45
27:A:2515:C:O2'	27:A:2516:A:H5'	2.16	0.45
54:4:52:ARG:CZ	54:4:54:VAL:HG12	2.47	0.45
1:a:336:A:O2'	1:a:337:G:H5'	2.17	0.45
1:a:399:G:H2'	1:a:400:C:C6	2.52	0.45
1:a:757:U:H2'	1:a:758:C:O4'	2.17	0.45
1:a:790:A:OP1	24:x:38:A:O2'	2.34	0.45
24:x:45:U:HO2'	24:x:46:G7M:P	2.40	0.45
26:z:143:ASP:OD1	26:z:145:GLU:N	2.50	0.45
27:A:1059:G:H2'	27:A:1060:U:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:76:PRO:HB2	31:E:84:THR:HG22	1.99	0.45
43:S:76:TYR:CZ	43:S:80:ILE:HG13	2.52	0.45
47:W:99:ASN:O	47:W:100:SER:C	2.59	0.45
52:2:8:THR:HA	52:2:34:HIS:O	2.17	0.45
8:h:75:ILE:HG23	8:h:75:ILE:O	2.17	0.44
27:A:1058:U:O2'	35:J:116:ASP:O	2.34	0.44
27:A:2185:U:C2	27:A:2186:G:C8	3.05	0.44
28:B:7:G:O2'	28:B:8:C:H5'	2.17	0.44
1:a:414:A:O2'	1:a:415:A:P	2.76	0.44
5:e:50:TYR:CE1	5:e:134:ILE:HD11	2.52	0.44
14:n:23:LYS:HA	14:n:26:GLU:HG2	1.99	0.44
27:A:146:A:HO2'	27:A:147:C:P	2.31	0.44
27:A:947:A:H2'	27:A:948:C:C6	2.53	0.44
27:A:1537:G:C2'	27:A:1538:G:O5'	2.65	0.44
27:A:2488:G:O2'	27:A:2489:U:H5'	2.17	0.44
37:M:43:ILE:HD12	37:M:56:ASP:HB2	2.00	0.44
1:a:1014:A:C2	1:a:1219:A:H1'	2.53	0.44
1:a:1071:C:H2'	1:a:1072:G:C8	2.53	0.44
3:c:47:LEU:HD21	3:c:87:LEU:HD11	1.98	0.44
4:d:95:GLU:O	4:d:100:ASN:ND2	2.47	0.44
4:d:105:MET:HE2	4:d:180:GLY:HA3	1.99	0.44
8:h:18:GLN:HG2	8:h:63:LEU:HD13	1.99	0.44
10:j:30:LYS:O	10:j:32:THR:N	2.50	0.44
27:A:207:A:H2'	27:A:208:C:O4'	2.18	0.44
27:A:609:A:H2'	27:A:610:C:O4'	2.16	0.44
27:A:819:A:C4	27:A:1189:A:C2	3.05	0.44
27:A:1496:A:H2'	27:A:1498:C:C5	2.52	0.44
27:A:1901:A:OP2	29:C:253:LYS:HE2	2.17	0.44
36:L:125:TYR:HH	36:L:132:HIS:CD2	2.35	0.44
41:Q:41:ALA:HB2	41:Q:48:LEU:HD21	1.99	0.44
41:Q:63:LYS:HG3	41:Q:64:TYR:N	2.33	0.44
43:S:58:ARG:HA	43:S:61:TRP:CE3	2.52	0.44
1:a:1032:G:H3'	1:a:1032:G:N3	2.31	0.44
4:d:60:LYS:NZ	4:d:195:ILE:HD13	2.32	0.44
8:h:5:ASP:OD2	8:h:81:PRO:HD3	2.17	0.44
29:C:155:ALA:HB2	29:C:162:VAL:HG23	1.99	0.44
53:3:12:ILE:HD11	53:3:24:ILE:HD11	2.00	0.44
1:a:1119:C:OP1	9:i:85:ARG:NH1	2.50	0.44
1:a:1477:U:H2'	1:a:1478:U:C6	2.52	0.44
6:f:67:PRO:HD2	6:f:70:VAL:HG11	2.00	0.44
10:j:80:THR:OG1	10:j:81:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:35:GLN:OE1	15:o:35:GLN:HA	2.17	0.44
17:q:12:VAL:HG22	17:q:21:ILE:HD12	2.00	0.44
27:A:131:A:H2'	27:A:132:G:C8	2.52	0.44
27:A:282:A:O2'	27:A:283:G:H5'	2.17	0.44
27:A:306:U:H2'	27:A:307:G:O4'	2.17	0.44
27:A:479:A:N3	27:A:481:G:H5''	2.32	0.44
27:A:1746:A:H2'	27:A:1747:U:C6	2.53	0.44
28:B:47:C:OP2	41:Q:3:LYS:NZ	2.50	0.44
51:l:7:ARG:HG3	51:l:56:LEU:HD22	1.99	0.44
1:a:593:U:H2'	1:a:594:U:C6	2.52	0.44
1:a:904:U:H2'	1:a:905:U:C6	2.53	0.44
5:e:14:LYS:HE3	5:e:116:GLU:CD	2.42	0.44
6:f:96:VAL:HG22	6:f:96:VAL:O	2.18	0.44
11:k:34:ILE:HG12	11:k:70:CYS:SG	2.57	0.44
26:z:94:THR:HG23	26:z:335:THR:HG22	2.00	0.44
27:A:608:A:H2'	27:A:609:A:C8	2.53	0.44
27:A:1081:U:C2	27:A:1082:U:C5	3.06	0.44
27:A:2233:U:H2'	27:A:2234:G:C8	2.52	0.44
28:B:114:C:O2'	28:B:115:A:H8	2.01	0.44
30:D:25:THR:HG23	30:D:189:VAL:HG22	2.00	0.44
1:a:2:A:H1'	1:a:613:C:O2'	2.18	0.44
1:a:98:A:O2'	1:a:99:C:H5'	2.17	0.44
1:a:458:U:H2'	1:a:459:A:C8	2.52	0.44
1:a:1285:A:H4'	1:a:1286:U:OP1	2.17	0.44
2:b:28:LYS:N	2:b:29:PRO:HD2	2.33	0.44
6:f:63:ASN:ND2	6:f:96:VAL:CG1	2.81	0.44
20:t:6:SER:O	20:t:10:ARG:HG2	2.18	0.44
26:z:141:VAL:HG11	26:z:147:LEU:CD1	2.48	0.44
27:A:191:A:H2'	27:A:192:C:C6	2.53	0.44
27:A:2557:G:H2'	27:A:2558:C:C6	2.52	0.44
27:A:2567:G:H2'	27:A:2568:U:C6	2.53	0.44
30:D:4:LEU:HD13	30:D:29:VAL:HG11	2.00	0.44
31:E:14:VAL:HB	31:E:197:GLU:OE2	2.17	0.44
31:E:130:LYS:HB2	31:E:133:LEU:HG	2.00	0.44
38:N:92:LEU:HD21	38:N:106:GLU:O	2.18	0.44
1:a:1004:A:H2'	1:a:1005:A:O4'	2.18	0.44
4:d:58:LYS:HA	4:d:200:ILE:CD1	2.47	0.44
10:j:9:ARG:NH1	10:j:71:LEU:HD21	2.33	0.44
26:z:208:ASP:OD2	26:z:208:ASP:N	2.41	0.44
27:A:279:A:N6	27:A:362:A:O4'	2.51	0.44
27:A:871:U:H2'	27:A:872:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1183:U:H2'	27:A:1184:U:C6	2.53	0.44
27:A:2178:C:H2'	27:A:2179:C:C5'	2.48	0.44
27:A:2522:U:O2'	27:A:2647:U:OP1	2.28	0.44
35:J:21:SER:O	35:J:25:GLY:N	2.37	0.44
18:r:22:ASP:OD1	18:r:25:ASP:HB2	2.17	0.44
23:w:50:C:O2'	23:w:51:G:P	2.76	0.44
27:A:1075:C:O2'	27:A:1076:C:OP1	2.34	0.44
41:Q:100:HIS:CG	41:Q:101:GLY:N	2.85	0.44
44:T:54:VAL:CG2	44:T:57:GLY:HA3	2.48	0.44
47:W:96:PHE:O	47:W:100:SER:HA	2.17	0.44
2:b:97:LEU:H	2:b:100:MET:HE3	1.84	0.43
26:z:121:LEU:HD21	26:z:125:GLN:HE21	1.83	0.43
27:A:53:A:H2'	27:A:54:G:O4'	2.17	0.43
27:A:286:U:H2'	27:A:287:G:C8	2.53	0.43
27:A:2271:G:OP1	49:Y:18:ALA:HB1	2.18	0.43
27:A:2857:G:N2	27:A:2860:A:OP2	2.34	0.43
41:Q:34:HIS:ND1	41:Q:53:THR:OG1	2.37	0.43
1:a:722:G:H5'	1:a:723:U:OP1	2.17	0.43
1:a:1410:A:H2'	1:a:1411:C:C6	2.53	0.43
2:b:83:ALA:O	2:b:87:CYS:HB2	2.18	0.43
27:A:282:A:OP2	27:A:282:A:H8	2.01	0.43
27:A:1721:G:C2'	27:A:1739:A:N6	2.81	0.43
27:A:2103:C:H2'	27:A:2104:C:H6	1.83	0.43
29:C:43:ARG:HA	29:C:48:ARG:O	2.18	0.43
1:a:144:G:H2'	1:a:145:G:O4'	2.18	0.43
5:e:14:LYS:HD2	5:e:117:VAL:CG1	2.48	0.43
10:j:8:ILE:HB	10:j:74:VAL:HG22	1.99	0.43
10:j:46:LYS:HB3	10:j:66:GLU:OE2	2.18	0.43
19:s:39:THR:HG23	19:s:41:PHE:CE1	2.52	0.43
27:A:279:A:C6	27:A:280:U:C4	3.07	0.43
27:A:588:U:H2'	27:A:589:U:C6	2.53	0.43
27:A:687:C:H2'	27:A:688:U:O4'	2.19	0.43
27:A:1061:U:H3'	27:A:1062:G:C5'	2.47	0.43
27:A:2280:G:O2'	27:A:2388:A:N1	2.50	0.43
29:C:2:ALA:N	29:C:20:VAL:O	2.51	0.43
1:a:429:U:H3'	4:d:9:LEU:HD12	1.99	0.43
2:b:15:HIS:HB3	2:b:43:LEU:CD1	2.49	0.43
19:s:50:ALA:HB1	19:s:57:HIS:HB3	2.00	0.43
27:A:247:G:H4'	27:A:386:G:C5	2.53	0.43
27:A:372:G:O2'	27:A:400:G:O6	2.29	0.43
27:A:881:G:O2'	27:A:896:A:N6	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2127:G:H2'	27:A:2128:G:C8	2.53	0.43
53:3:36:VAL:CG1	53:3:41:HIS:HB2	2.47	0.43
1:a:568:G:O2'	1:a:574:A:N1	2.44	0.43
1:a:713:G:H2'	1:a:714:G:C8	2.54	0.43
1:a:1036:A:H2'	1:a:1037:C:C5'	2.49	0.43
27:A:176:A:O2'	27:A:177:G:H5'	2.18	0.43
27:A:454:A:H4'	27:A:455:C:OP2	2.18	0.43
27:A:1796:U:H2'	27:A:1797:G:H8	1.82	0.43
27:A:2189:U:H4'	27:A:2190:G:OP1	2.19	0.43
36:L:92:MET:HE3	36:L:92:MET:HB3	1.93	0.43
37:M:18:ARG:HB2	37:M:45:GLU:HG2	1.99	0.43
38:N:82:LEU:HD22	38:N:90:VAL:HG21	2.01	0.43
46:V:4:GLU:HG3	46:V:49:LYS:HE3	2.01	0.43
1:a:1287:A:H2'	1:a:1288:A:C8	2.54	0.43
2:b:54:LEU:HB3	2:b:220:THR:HG21	2.00	0.43
7:g:129:GLU:OE2	7:g:129:GLU:C	2.61	0.43
8:h:96:MET:HE3	8:h:99:LEU:HB2	2.00	0.43
27:A:75:G:N3	27:A:75:G:H2'	2.33	0.43
27:A:147:C:O2'	27:A:148:U:P	2.76	0.43
27:A:340:A:H2'	27:A:341:C:O4'	2.19	0.43
27:A:1720:U:H2'	27:A:1721:G:O4'	2.17	0.43
27:A:2036:C:O5'	27:A:2036:C:O2	2.36	0.43
27:A:2480:C:H2'	27:A:2481:G:H5'	2.01	0.43
29:C:115:GLN:O	29:C:125:LYS:HE3	2.19	0.43
1:a:244:U:O4	1:a:906:A:H1'	2.17	0.43
1:a:1404:C:H2'	1:a:1405:G:C8	2.54	0.43
2:b:167:ASP:HB2	2:b:191:SER:OG	2.19	0.43
27:A:529:A:H4'	27:A:530:G:OP1	2.18	0.43
27:A:708:G:O2'	27:A:709:U:H5'	2.18	0.43
27:A:1048:A:C5	27:A:1049:C:C5	3.06	0.43
38:N:123:ARG:NH1	38:N:143:GLU:OE2	2.47	0.43
41:Q:76:LYS:O	41:Q:80:GLU:HG3	2.19	0.43
1:a:921:U:H2'	1:a:922:G:O4'	2.17	0.43
2:b:173:ILE:HD12	2:b:183:VAL:HG11	2.01	0.43
27:A:26:G:H1'	27:A:514:A:N6	2.34	0.43
27:A:1607:C:H4'	27:A:1608:A:O5'	2.19	0.43
27:A:2680:U:O2'	27:A:2681:C:H5'	2.19	0.43
33:G:105:LEU:HD11	33:G:148:LEU:HD22	2.01	0.43
52:2:4:THR:CB	52:2:37:GLU:OE2	2.67	0.43
1:a:269:C:H2'	1:a:270:A:C8	2.53	0.43
3:c:129:MET:SD	3:c:131:ARG:HB2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:83:LEU:HD11	19:s:66:MET:HB3	1.99	0.43
23:w:66:U:H2'	23:w:67:U:H6	1.84	0.43
24:x:75:C:H2'	24:x:76:A:O4'	2.19	0.43
27:A:12:U:O2'	27:A:13:A:C8	2.70	0.43
27:A:527:C:H4'	27:A:528:A:O5'	2.18	0.43
27:A:544:C:O3'	27:A:545:U:C6	2.71	0.43
27:A:722:A:H2'	27:A:723:C:O4'	2.19	0.43
27:A:888:C:H2'	27:A:889:C:O4'	2.18	0.43
27:A:1064:C:O2'	27:A:1065:U:H5''	2.19	0.43
27:A:1427:A:H4'	27:A:1428:C:O4'	2.18	0.43
27:A:2480:C:C2'	27:A:2481:G:H5'	2.49	0.43
27:A:2649:C:H2'	27:A:2650:U:H6	1.83	0.43
1:a:56:U:H2'	1:a:57:G:C8	2.54	0.43
1:a:278:G:OP2	17:q:43:LYS:NZ	2.47	0.43
1:a:1163:A:H2'	1:a:1164:G:O4'	2.19	0.43
1:a:1412:C:H2'	1:a:1413:A:C8	2.54	0.43
27:A:624:C:O2'	27:A:657:U:OP1	2.35	0.43
28:B:114:C:HO2'	28:B:115:A:P	2.42	0.43
30:D:152:PRO:HG3	30:D:156:PHE:CZ	2.54	0.43
33:G:43:VAL:HG23	33:G:50:LEU:HD22	2.01	0.43
1:a:1513:A:H2'	1:a:1514:G:C8	2.54	0.42
2:b:111:ILE:HD12	2:b:152:LYS:HA	2.01	0.42
3:c:105:GLU:OE2	3:c:106:VAL:N	2.52	0.42
10:j:15:HIS:HA	10:j:18:ILE:HG22	2.01	0.42
23:w:6:A:O2'	23:w:7:A:H5'	2.19	0.42
27:A:182:A:H2'	27:A:183:C:H6	1.83	0.42
27:A:278:A:N6	27:A:362:A:C8	2.86	0.42
27:A:930:G:H1'	52:2:25:LEU:HD11	2.00	0.42
27:A:1542:U:O2'	27:A:1543:G:H5'	2.19	0.42
27:A:1902:C:H4'	29:C:242:LYS:O	2.19	0.42
27:A:1903:G:OP2	64:A:3803:HOH:O	2.22	0.42
27:A:2646:C:H2'	27:A:2647:U:O4'	2.18	0.42
27:A:2662:A:H2'	27:A:2663:G:O4'	2.19	0.42
27:A:2839:G:O2'	40:P:49:GLU:OE1	2.30	0.42
27:A:2847:U:H2'	27:A:2848:G:O4'	2.19	0.42
1:a:1:A:H2'	1:a:2:A:O5'	2.19	0.42
12:l:110:ARG:HB3	12:l:119:VAL:HG21	2.01	0.42
26:z:283:LYS:HB2	26:z:286:GLU:HG3	2.01	0.42
27:A:419:U:H2'	27:A:420:C:C6	2.54	0.42
27:A:528:A:O2'	27:A:529:A:H5'	2.18	0.42
27:A:544:C:H5'	27:A:545:U:OP2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1269:A:H2'	27:A:1270:C:C6	2.54	0.42
46:V:5:GLU:H	46:V:5:GLU:CD	2.26	0.42
1:a:58:C:O2'	1:a:388:G:N7	2.43	0.42
2:b:9:MET:HB3	2:b:43:LEU:HD21	2.01	0.42
5:e:15:LEU:C	5:e:15:LEU:HD13	2.44	0.42
8:h:54:ASP:OD1	8:h:55:THR:N	2.52	0.42
9:i:7:TYR:HE1	9:i:18:ARG:HB3	1.85	0.42
9:i:116:VAL:HG11	10:j:62:ARG:HG3	2.01	0.42
27:A:299:A:N3	27:A:319:G:O2'	2.36	0.42
27:A:1080:A:H2'	27:A:1081:U:O5'	2.19	0.42
27:A:2687:U:H2'	27:A:2688:G:O4'	2.18	0.42
44:T:34:GLU:OE1	44:T:60:LYS:HE3	2.19	0.42
9:i:6:TYR:CE1	9:i:90:TYR:CD1	3.07	0.42
27:A:541:A:H2'	27:A:542:C:O4'	2.20	0.42
27:A:1066:U:O2'	27:A:1068:G:N7	2.38	0.42
28:B:3:C:O2'	28:B:4:C:O5'	2.36	0.42
28:B:42:C:C6	32:F:66:LEU:HB2	2.55	0.42
1:a:542:G:H5'	4:d:39:GLY:HA3	2.02	0.42
3:c:21:THR:OG1	3:c:58:GLU:HG2	2.20	0.42
18:r:42:SER:OG	18:r:47:THR:O	2.38	0.42
26:z:343:GLU:O	26:z:344:LEU:C	2.63	0.42
27:A:287:G:H2'	27:A:288:U:C6	2.54	0.42
27:A:549:G:H2'	27:A:550:C:H6	1.84	0.42
27:A:832:U:H2'	27:A:833:A:C8	2.55	0.42
27:A:1858:A:H2'	27:A:1859:U:O4'	2.20	0.42
27:A:2520:C:C6	27:A:2567:G:H1'	2.54	0.42
28:B:30:C:H2'	28:B:31:C:H5'	2.01	0.42
28:B:48:U:H4'	41:Q:100:HIS:CD2	2.54	0.42
41:Q:88:LYS:HE2	41:Q:88:LYS:HB3	1.91	0.42
43:S:105:ALA:HA	44:T:47:VAL:HG21	2.00	0.42
1:a:867:G:O2'	1:a:873:A:N1	2.50	0.42
1:a:1141:C:O2'	1:a:1142:G:H5'	2.19	0.42
2:b:68:LEU:HB3	2:b:161:LEU:HD12	2.01	0.42
5:e:41:ASP:OD1	5:e:41:ASP:O	2.38	0.42
26:z:388:VAL:HG22	26:z:389:VAL:N	2.33	0.42
27:A:84:A:H4'	27:A:85:G:O5'	2.20	0.42
27:A:848:C:H2'	27:A:849:A:C8	2.54	0.42
27:A:1084:A:C2'	27:A:1085:A:O5'	2.64	0.42
27:A:1110:G:C2'	27:A:1111:A:OP2	2.68	0.42
27:A:1750:G:O2'	27:A:2860:A:N1	2.44	0.42
27:A:1799:G:O2'	29:C:180:GLU:OE2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2070:A:H2'	27:A:2071:A:O4'	2.20	0.42
27:A:2615:U:C2	54:4:4:GLN:HA	2.55	0.42
38:N:1:MET:O	38:N:1:MET:HG3	2.19	0.42
39:O:38:ARG:HB2	39:O:98:PRO:HD3	2.01	0.42
39:O:111:GLU:OE2	39:O:111:GLU:HA	2.19	0.42
47:W:98:SER:O	47:W:99:ASN:CG	2.62	0.42
50:Z:41:GLU:OE1	50:Z:41:GLU:O	2.37	0.42
1:a:178:C:C2	1:a:179:A:C8	3.08	0.42
1:a:1023:U:H2'	1:a:1024:G:H8	1.85	0.42
6:f:39:LEU:HD13	6:f:39:LEU:C	2.44	0.42
39:O:47:GLU:OE2	39:O:51:ARG:NE	2.53	0.42
53:3:16:CYS:SG	53:3:17:SER:N	2.92	0.42
1:a:414:A:H2'	1:a:415:A:O4'	2.19	0.42
1:a:923:A:O2'	1:a:1399:C:OP2	2.30	0.42
1:a:1004:A:C2	1:a:1026:G:N2	2.88	0.42
1:a:1394:A:N1	1:a:1500:A:O2'	2.44	0.42
13:m:4:ILE:HG23	13:m:57:ARG:HG2	2.01	0.42
27:A:150:U:H2'	27:A:151:C:C6	2.55	0.42
27:A:909:A:H2'	27:A:912:C:C5	2.55	0.42
27:A:1139:G:O3'	36:L:26:GLY:HA3	2.19	0.42
27:A:2669:G:H3'	27:A:2670:A:H5''	2.02	0.42
1:a:33:A:H2'	1:a:34:C:C6	2.55	0.42
1:a:662:U:H2'	1:a:663:A:C8	2.55	0.42
2:b:212:LEU:C	2:b:212:LEU:HD23	2.45	0.42
26:z:85:HIS:ND1	26:z:85:HIS:N	2.68	0.42
26:z:379:GLU:CG	26:z:380:GLY:H	2.32	0.42
27:A:848:C:H2'	27:A:849:A:H8	1.85	0.42
27:A:1641:A:H2'	27:A:1642:G:O4'	2.20	0.42
27:A:2101:A:C2	27:A:2102:G:C8	3.08	0.42
29:C:78:VAL:HG21	29:C:110:LEU:HD21	2.00	0.42
31:E:173:THR:HA	31:E:199:MET:HE1	2.01	0.42
45:U:29:VAL:HB	45:U:55:ILE:HD11	2.02	0.42
1:a:96:U:H1'	1:a:97:G:OP1	2.19	0.42
27:A:243:U:OP1	57:7:6:THR:HG21	2.20	0.42
27:A:1411:U:O2'	27:A:1412:U:H5'	2.19	0.42
27:A:2698:U:H2'	27:A:2699:C:C6	2.55	0.42
42:R:33:VAL:HG22	42:R:38:LYS:HB3	2.01	0.42
53:3:12:ILE:N	53:3:24:ILE:O	2.45	0.42
1:a:438:U:O2'	1:a:439:U:C5	2.73	0.41
1:a:1019:A:H2'	1:a:1020:G:O4'	2.19	0.41
5:e:13:GLU:O	5:e:14:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:115:LEU:HD13	5:e:123:VAL:HG11	2.02	0.41
10:j:67:ILE:HG13	14:n:96:LEU:HD12	2.02	0.41
27:A:499:U:H2'	27:A:500:G:O4'	2.20	0.41
27:A:1106:G:C4	27:A:1107:G:C8	3.08	0.41
27:A:1484:U:O2'	27:A:1485:U:H5'	2.20	0.41
27:A:2262:U:OP1	27:A:2387:U:O2'	2.32	0.41
1:a:997:U:H2'	1:a:998:C:O4'	2.20	0.41
1:a:1123:U:O2'	1:a:1124:G:H5'	2.20	0.41
1:a:1179:A:H2'	1:a:1180:A:O4'	2.19	0.41
23:w:16:H2U:OP2	23:w:16:H2U:H3'	2.21	0.41
27:A:645:C:H2'	27:A:647:G:C8	2.56	0.41
27:A:721:A:H2'	27:A:722:A:C8	2.55	0.41
27:A:1110:G:O2'	27:A:1111:A:O5'	2.38	0.41
27:A:1177:G:H2'	27:A:1178:C:C6	2.55	0.41
28:B:48:U:H2'	28:B:49:C:C6	2.55	0.41
31:E:176:ASP:CG	31:E:179:SER:HG	2.27	0.41
40:P:117:ASP:OD1	40:P:117:ASP:C	2.62	0.41
47:W:39:ILE:HG22	47:W:40:ASN:N	2.35	0.41
1:a:580:C:H2'	1:a:581:G:O4'	2.20	0.41
1:a:977:A:O2'	1:a:979:C:OP2	2.36	0.41
3:c:88:ARG:CZ	3:c:88:ARG:HB3	2.50	0.41
27:A:1064:C:O2'	27:A:1065:U:C5'	2.68	0.41
27:A:1563:U:H2'	27:A:1564:C:C6	2.55	0.41
27:A:1847:A:H1'	27:A:1848:A:N7	2.36	0.41
27:A:2020:A:H5'	54:4:9:THR:CG2	2.50	0.41
35:J:107:GLN:CB	35:J:110:ALA:HB2	2.50	0.41
39:O:26:VAL:HG13	39:O:104:GLU:HG2	2.02	0.41
43:S:104:VAL:HG11	44:T:45:GLU:HG3	2.02	0.41
45:U:65:ASP:OD1	45:U:67:ASP:OD1	2.37	0.41
1:a:1476:A:H2'	1:a:1477:U:O4'	2.20	0.41
23:w:26:A:C2	23:w:44:G:N1	2.89	0.41
27:A:92:U:H2'	27:A:93:G:O4'	2.21	0.41
27:A:1064:C:H4'	35:J:90:SER:O	2.21	0.41
27:A:1530:G:H2'	27:A:1531:C:O4'	2.19	0.41
27:A:1857:G:HO2'	27:A:1858:A:H8	1.65	0.41
27:A:2014:A:H2'	27:A:2015:A:C8	2.55	0.41
27:A:2637:U:C2'	27:A:2638:G:H5'	2.50	0.41
27:A:2752:C:H2'	27:A:2753:A:O4'	2.20	0.41
31:E:120:VAL:HA	31:E:188:MET:O	2.20	0.41
33:G:96:ALA:N	33:G:128:GLN:O	2.49	0.41
39:O:50:ARG:HD3	39:O:65:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:136:MET:HE2	48:X:77:VAL:HG23	2.01	0.41
52:2:10:THR:HG22	52:2:56:LYS:HE3	2.02	0.41
1:a:389:A:H3'	1:a:390:U:H6	1.85	0.41
1:a:918:A:H2'	1:a:919:A:O4'	2.21	0.41
6:f:67:PRO:O	6:f:70:VAL:HG12	2.20	0.41
16:p:61:VAL:HG21	16:p:67:ILE:HD11	2.01	0.41
27:A:160:A:N3	27:A:2208:C:O2'	2.46	0.41
27:A:718:A:H2'	27:A:719:C:H5'	2.02	0.41
27:A:877:A:N6	27:A:899:A:C5	2.89	0.41
27:A:1085:A:H2'	27:A:1086:A:C4	2.55	0.41
27:A:1590:A:H2'	27:A:1591:A:C8	2.55	0.41
27:A:1599:U:H2'	27:A:1600:C:C6	2.56	0.41
27:A:1715:G:N2	27:A:1744:A:OP2	2.44	0.41
27:A:1923:U:H2'	27:A:1924:C:C6	2.56	0.41
27:A:2135:A:HO2'	27:A:2159:G:HO2'	1.65	0.41
27:A:2246:G:H2'	27:A:2247:A:C8	2.56	0.41
28:B:119:A:C2'	28:B:120:U:O5'	2.67	0.41
49:Y:56:ASP:OD1	49:Y:58:THR:OG1	2.36	0.41
56:6:45:SER:O	56:6:46:LYS:CB	2.68	0.41
1:a:195:A:C2'	1:a:196:A:O5'	2.68	0.41
1:a:216:U:H2'	1:a:217:C:C6	2.56	0.41
1:a:1191:A:OP1	3:c:4:LYS:NZ	2.43	0.41
1:a:1287:A:N3	1:a:1353:G:O2'	2.41	0.41
27:A:414:C:H2'	27:A:415:A:C8	2.55	0.41
27:A:418:C:H2'	27:A:419:U:O4'	2.20	0.41
27:A:580:U:H2'	27:A:581:C:C6	2.56	0.41
27:A:993:G:OP2	43:S:51:ARG:NH2	2.52	0.41
27:A:1330:C:O2'	27:A:1331:G:H5'	2.20	0.41
27:A:2419:U:H4'	55:5:22:THR:HG21	2.01	0.41
1:a:982:U:H4'	1:a:983:A:O4'	2.21	0.41
1:a:983:A:H5'	1:a:984:C:OP2	2.21	0.41
2:b:163:VAL:HG13	2:b:169:GLU:HG3	2.03	0.41
4:d:197:GLU:CD	4:d:197:GLU:H	2.28	0.41
5:e:15:LEU:HD11	5:e:18:VAL:HG23	2.02	0.41
6:f:10:VAL:HG11	6:f:18:VAL:HG22	2.02	0.41
11:k:87:LYS:HB3	11:k:113:VAL:HG23	2.02	0.41
23:w:66:U:H2'	23:w:67:U:C6	2.55	0.41
26:z:322:PRO:HG3	26:z:350:MET:HE3	2.02	0.41
27:A:555:G:O2'	27:A:556:A:H8	2.04	0.41
27:A:717:C:O2	27:A:717:C:O4'	2.37	0.41
27:A:851:C:H2'	27:A:852:U:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2144:G:O6	27:A:2148:G:O6	2.38	0.41
27:A:2467:C:OP1	58:8:8:LYS:NZ	2.53	0.41
49:Y:37:ILE:HG21	49:Y:80:ILE:HG21	2.01	0.41
57:7:31:HIS:CD2	57:7:32:ILE:H	2.39	0.41
1:a:49:U:O2'	1:a:50:A:H2'	2.21	0.41
1:a:539:A:H2'	1:a:540:G:C8	2.56	0.41
1:a:827:U:H2'	1:a:870:U:O4	2.20	0.41
1:a:1130:A:C4	1:a:1131:G:C8	3.08	0.41
3:c:206:GLU:O	3:c:207:ILE:HG12	2.21	0.41
10:j:6:ILE:HD13	10:j:102:LEU:HG	2.02	0.41
14:n:19:LYS:HG3	14:n:20:TYR:CD1	2.56	0.41
62:z:402:MQH:N03	62:z:402:MQH:C55	2.83	0.41
27:A:1080:A:H2'	27:A:1080:A:N3	2.36	0.41
27:A:1601:G:O2'	27:A:1602:U:H5'	2.21	0.41
1:a:505:G:C6	1:a:535:A:C2	3.09	0.41
1:a:559:A:H4'	1:a:560:A:H3'	2.03	0.41
1:a:1451:U:C2'	1:a:1452:C:OP1	2.69	0.41
2:b:8:ASP:O	2:b:12:ALA:N	2.53	0.41
5:e:11:LEU:HD13	5:e:39:VAL:CG1	2.51	0.41
5:e:22:SER:HB3	5:e:31:PHE:CD1	2.56	0.41
6:f:74:LEU:HA	6:f:77:THR:HG22	2.02	0.41
8:h:13:ARG:NH1	8:h:26:THR:O	2.54	0.41
19:s:12:ASP:OD1	19:s:35:SER:CB	2.69	0.41
26:z:268:GLU:O	26:z:269:GLY:C	2.63	0.41
27:A:279:A:N6	27:A:362:A:C4'	2.84	0.41
27:A:570:G:H2'	27:A:2030:6MZ:N7	2.36	0.41
27:A:657:U:H2'	27:A:658:U:C6	2.56	0.41
27:A:849:A:H2'	27:A:850:U:H6	1.84	0.41
27:A:1315:C:O2'	27:A:1392:A:N3	2.45	0.41
27:A:2182:U:H2'	27:A:2183:A:C8	2.55	0.41
27:A:2756:U:H4'	27:A:2757:A:OP1	2.20	0.41
27:A:2812:G:H2'	27:A:2813:A:O4'	2.21	0.41
28:B:57:A:H4'	32:F:27:GLN:OE1	2.21	0.41
29:C:20:VAL:O	29:C:20:VAL:HG23	2.21	0.41
32:F:29:PRO:HG3	32:F:165:GLU:HG3	2.03	0.41
47:W:10:GLU:OE1	47:W:73:PHE:HB3	2.21	0.41
1:a:1160:G:C5	1:a:1161:C:C5	3.09	0.41
1:a:1330:U:H2'	1:a:1331:G:O4'	2.20	0.41
2:b:135:LEU:O	2:b:138:THR:OG1	2.34	0.41
4:d:94:LEU:O	4:d:97:ARG:HG2	2.21	0.41
9:i:50:GLN:OE1	9:i:80:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:64:GLN:HG3	11:k:68:GLU:OE2	2.21	0.41
23:w:11:C:H2'	23:w:12:U:C6	2.56	0.41
26:z:29:THR:HG23	26:z:79:HIS:CD2	2.56	0.41
26:z:141:VAL:CG1	26:z:147:LEU:HD13	2.51	0.41
27:A:1505:A:H2'	27:A:1506:U:C6	2.56	0.41
27:A:1549:A:H2'	27:A:1550:C:O4'	2.21	0.41
27:A:1747:U:H2'	27:A:1748:C:C6	2.56	0.41
27:A:2395:C:H2'	27:A:2396:G:O4'	2.21	0.41
27:A:2828:G:O2'	27:A:2829:A:H5'	2.20	0.41
40:P:29:VAL:O	40:P:78:LYS:NZ	2.50	0.41
46:V:30:ILE:HG13	46:V:85:VAL:HB	2.02	0.41
1:a:1226:C:H4'	19:s:80:TYR:CZ	2.55	0.40
6:f:37:HIS:O	6:f:97:THR:HG23	2.21	0.40
7:g:27:VAL:HG22	7:g:43:VAL:HG21	2.03	0.40
26:z:151:GLU:OE2	26:z:170:ILE:HG21	2.21	0.40
27:A:287:G:H2'	27:A:288:U:H6	1.85	0.40
27:A:2173:A:H2'	27:A:2174:C:C6	2.56	0.40
27:A:2723:C:H2'	27:A:2724:U:O4'	2.21	0.40
28:B:24:G:N7	28:B:56:G:H2'	2.36	0.40
28:B:119:A:H2'	28:B:120:U:O4'	2.21	0.40
31:E:108:ILE:HG23	38:N:1:MET:HE1	2.03	0.40
1:a:57:G:H2'	1:a:58:C:C6	2.56	0.40
1:a:177:G:C5	1:a:178:C:C5	3.09	0.40
1:a:463:U:O3'	1:a:464:U:O4'	2.39	0.40
2:b:123:ASP:O	2:b:123:ASP:OD1	2.39	0.40
5:e:77:ASN:O	5:e:77:ASN:CG	2.64	0.40
27:A:151:C:H2'	27:A:152:A:C8	2.56	0.40
27:A:360:U:H2'	27:A:361:G:O4'	2.20	0.40
27:A:428:A:O2'	27:A:429:A:H5'	2.21	0.40
27:A:1210:G:OP1	27:A:1211:C:O2'	2.36	0.40
27:A:2063:C:O2	27:A:2450:A:N1	2.55	0.40
27:A:2298:A:OP1	32:F:71:ARG:HD2	2.21	0.40
27:A:2572:A:C4'	27:A:2573:C:OP2	2.69	0.40
27:A:2809:A:H2'	27:A:2810:A:C8	2.57	0.40
47:W:74:ASN:O	47:W:75:ALA:HB3	2.21	0.40
1:a:412:A:O2'	1:a:414:A:H5'	2.20	0.40
1:a:882:C:O2'	1:a:883:C:H5'	2.21	0.40
1:a:1158:C:C5	1:a:1160:G:H1'	2.55	0.40
1:a:1407:5MC:O2'	27:A:1912:A:N1	2.52	0.40
1:a:1448:C:O2'	1:a:1449:C:H6	2.04	0.40
15:o:80:GLN:HE21	15:o:80:GLN:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:x:65:G:H2'	24:x:66:U:C6	2.56	0.40
26:z:131:ILE:HD12	26:z:163:PHE:CE1	2.57	0.40
27:A:78:U:H2'	27:A:79:C:C6	2.55	0.40
27:A:223:A:N1	27:A:407:G:O2'	2.50	0.40
27:A:355:U:H2'	27:A:356:G:O4'	2.21	0.40
27:A:1103:A:H2'	27:A:1104:C:OP1	2.21	0.40
27:A:1275:A:N1	27:A:1295:C:O2'	2.49	0.40
27:A:1357:C:H2'	27:A:1358:G:O4'	2.21	0.40
27:A:1470:A:H2'	27:A:1471:G:O4'	2.20	0.40
27:A:2125:G:H2'	27:A:2126:A:O4'	2.20	0.40
27:A:2297:A:C2	27:A:2320:U:O4'	2.74	0.40
27:A:2700:A:H2'	27:A:2701:U:C6	2.57	0.40
27:A:2800:A:C2	27:A:2895:G:H1'	2.56	0.40
33:G:125:CYS:SG	33:G:131:ILE:HG22	2.60	0.40
36:L:10:THR:HG22	36:L:10:THR:O	2.21	0.40
1:a:94:G:H4'	1:a:95:C:H5'	2.03	0.40
1:a:134:G:H1'	1:a:325:A:C5	2.56	0.40
1:a:161:A:H2'	1:a:162:A:C8	2.57	0.40
1:a:459:A:H2'	1:a:460:A:C8	2.56	0.40
1:a:1206:G:H2'	1:a:1207:2MG:O4'	2.21	0.40
1:a:1449:C:O2'	1:a:1450:U:P	2.80	0.40
4:d:156:LYS:O	4:d:160:GLU:OE1	2.38	0.40
22:v:27:C:H2'	22:v:28:G:O4'	2.21	0.40
25:y:104:LYS:HG3	27:A:2506:U:O4	2.21	0.40
27:A:518:G:H2'	27:A:519:U:C6	2.57	0.40
27:A:641:U:O2'	27:A:2350:C:OP1	2.38	0.40
27:A:780:G:H2'	27:A:782:A:N7	2.37	0.40
27:A:1199:U:H2'	27:A:1200:C:H6	1.86	0.40
27:A:1672:A:C2	27:A:2582:G:H5'	2.56	0.40
27:A:2135:A:N3	27:A:2135:A:H2'	2.36	0.40
31:E:9:GLN:HG3	31:E:9:GLN:O	2.21	0.40
36:L:110:PRO:O	36:L:115:GLY:HA3	2.21	0.40
1:a:1251:A:H2'	1:a:1252:A:O4'	2.20	0.40
1:a:1316:G:O2'	1:a:1318:A:N7	2.51	0.40
6:f:6:ILE:HG12	6:f:89:VAL:HG22	2.03	0.40
11:k:44:TRP:HA	11:k:70:CYS:SG	2.62	0.40
26:z:182:ASP:O	26:z:186:GLU:HG3	2.21	0.40
27:A:1211:C:H3'	27:A:1212:G:H5'	2.03	0.40
27:A:1465:G:O2'	27:A:1545:A:N1	2.52	0.40
27:A:2000:C:OP1	40:P:5:LYS:NZ	2.43	0.40
27:A:2093:G:OP1	64:A:3804:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2202:U:O2'	27:A:2204:G:OP1	2.35	0.40
30:D:38:LYS:NZ	30:D:81:GLU:OE2	2.40	0.40
48:X:21:ARG:HA	48:X:25:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	c	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
4	d	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	e	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
6	f	101/131 (77%)	97 (96%)	4 (4%)	0	100	100
7	g	150/156 (96%)	140 (93%)	10 (7%)	0	100	100
8	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	i	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	j	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	12	8
11	k	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	l	118/124 (95%)	116 (98%)	2 (2%)	0	100	100
13	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	n	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	p	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	r	52/75 (69%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	u	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
25	y	1/3 (33%)	0	1 (100%)	0	100	100
26	z	367/394 (93%)	340 (93%)	27 (7%)	0	100	100
29	C	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
30	D	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	21
31	E	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
32	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
33	G	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
34	H	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
35	J	139/142 (98%)	119 (86%)	19 (14%)	1 (1%)	18	14
36	L	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
37	M	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
38	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
39	O	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
40	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
41	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	R	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	S	115/118 (98%)	115 (100%)	0	0	100	100
44	T	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
45	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	V	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
47	W	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
48	X	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
49	Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
50	Z	75/78 (96%)	75 (100%)	0	0	100	100
51	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
52	2	56/59 (95%)	56 (100%)	0	0	100	100
53	3	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
54	4	53/57 (93%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	5	49/55 (89%)	49 (100%)	0	0	100	100
56	6	44/46 (96%)	44 (100%)	0	0	100	100
57	7	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
58	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5968/6425 (93%)	5743 (96%)	222 (4%)	3 (0%)	49	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	J	33	VAL
10	j	57	VAL
30	D	149	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	186/199 (94%)	180 (97%)	6 (3%)	34	35
3	c	170/190 (90%)	163 (96%)	7 (4%)	27	26
4	d	172/173 (99%)	167 (97%)	5 (3%)	37	40
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	84 (93%)	6 (7%)	15	11
7	g	125/129 (97%)	120 (96%)	5 (4%)	28	27
8	h	104/105 (99%)	103 (99%)	1 (1%)	68	75
9	i	105/107 (98%)	101 (96%)	4 (4%)	29	29
10	j	86/90 (96%)	84 (98%)	2 (2%)	44	49
11	k	89/98 (91%)	88 (99%)	1 (1%)	65	73
12	l	101/103 (98%)	100 (99%)	1 (1%)	68	75
13	m	93/96 (97%)	92 (99%)	1 (1%)	65	73
14	n	83/84 (99%)	82 (99%)	1 (1%)	63	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	o	76/77 (99%)	75 (99%)	1 (1%)	61	68
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	37
17	q	73/78 (94%)	72 (99%)	1 (1%)	59	66
18	r	47/65 (72%)	45 (96%)	2 (4%)	26	25
19	s	72/79 (91%)	71 (99%)	1 (1%)	59	66
20	t	65/66 (98%)	62 (95%)	3 (5%)	24	22
21	u	60/61 (98%)	59 (98%)	1 (2%)	53	60
25	y	3/3 (100%)	3 (100%)	0	100	100
26	z	312/327 (95%)	305 (98%)	7 (2%)	45	50
29	C	216/218 (99%)	213 (99%)	3 (1%)	59	66
30	D	163/163 (100%)	161 (99%)	2 (1%)	63	70
31	E	165/165 (100%)	162 (98%)	3 (2%)	51	58
32	F	148/150 (99%)	143 (97%)	5 (3%)	32	33
33	G	137/138 (99%)	132 (96%)	5 (4%)	31	31
34	H	32/114 (28%)	31 (97%)	1 (3%)	35	37
36	L	116/116 (100%)	115 (99%)	1 (1%)	70	78
37	M	104/104 (100%)	103 (99%)	1 (1%)	68	75
38	N	103/103 (100%)	100 (97%)	3 (3%)	37	40
39	O	107/107 (100%)	107 (100%)	0	100	100
40	P	98/103 (95%)	98 (100%)	0	100	100
41	Q	86/87 (99%)	81 (94%)	5 (6%)	18	15
42	R	99/100 (99%)	97 (98%)	2 (2%)	48	54
43	S	89/90 (99%)	89 (100%)	0	100	100
44	T	84/84 (100%)	82 (98%)	2 (2%)	43	47
45	U	93/93 (100%)	93 (100%)	0	100	100
46	V	80/84 (95%)	80 (100%)	0	100	100
47	W	83/85 (98%)	79 (95%)	4 (5%)	23	21
48	X	78/78 (100%)	76 (97%)	2 (3%)	40	44
49	Y	57/63 (90%)	57 (100%)	0	100	100
50	Z	67/68 (98%)	66 (98%)	1 (2%)	57	64
51	1	54/55 (98%)	53 (98%)	1 (2%)	50	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	2	48/49 (98%)	47 (98%)	1 (2%)	47	52
53	3	54/62 (87%)	50 (93%)	4 (7%)	13	9
54	4	46/48 (96%)	46 (100%)	0	100	100
55	5	46/49 (94%)	45 (98%)	1 (2%)	45	50
56	6	37/38 (97%)	37 (100%)	0	100	100
57	7	51/52 (98%)	51 (100%)	0	100	100
58	8	34/34 (100%)	33 (97%)	1 (3%)	37	40
All	All	4871/5133 (95%)	4765 (98%)	106 (2%)	45	50

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	6	MET
2	b	38	VAL
2	b	119	THR
2	b	138	THR
2	b	164	ILE
2	b	196	VAL
3	c	35	SER
3	c	45	LYS
3	c	66	VAL
3	c	67	THR
3	c	88	ARG
3	c	177	THR
3	c	207	ILE
4	d	68	LEU
4	d	137	VAL
4	d	160	GLU
4	d	189	SER
4	d	205	SER
6	f	15	SER
6	f	22	ILE
6	f	54	LEU
6	f	61	LEU
6	f	94	HIS
6	f	102	MET
7	g	37	SER
7	g	54	SER
7	g	72	THR
7	g	75	VAL

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Mol	Chain	Res	Type
7	g	83	SER
8	h	107	SER
9	i	15	SER
9	i	55	VAL
9	i	58	VAL
9	i	128	SER
10	j	10	LEU
10	j	80	THR
11	k	17	SER
12	l	4	VAL
13	m	65	VAL
14	n	31	ILE
15	o	45	GLU
16	p	21	VAL
16	p	63	GLN
17	q	43	LYS
18	r	47	THR
18	r	66	SER
19	s	4	SER
20	t	6	SER
20	t	49	LYS
20	t	82	GLN
21	u	51	SER
26	z	13	VAL
26	z	74	THR
26	z	325	LYS
26	z	344	LEU
26	z	359	MET
26	z	379	GLU
26	z	393	LEU
29	C	38	SER
29	C	65	VAL
29	C	118	SER
30	D	1	MET
30	D	97	SER
31	E	84	THR
31	E	126	VAL
31	E	166	LYS
32	F	73	SER
32	F	89	VAL
32	F	104	ILE
32	F	135	GLN

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Mol	Chain	Res	Type
32	F	175	PHE
33	G	9	VAL
33	G	15	VAL
33	G	34	THR
33	G	106	SER
33	G	155	GLU
34	H	17	ASP
36	L	3	THR
37	M	66	LYS
38	N	116	VAL
38	N	120	VAL
38	N	144	GLU
41	Q	19	GLN
41	Q	24	THR
41	Q	35	ILE
41	Q	62	LEU
41	Q	78	VAL
42	R	78	SER
42	R	114	LEU
44	T	45	GLU
44	T	54	VAL
47	W	39	ILE
47	W	46	GLN
47	W	81	ASP
47	W	83	VAL
48	X	8	VAL
48	X	65	VAL
50	Z	42	SER
51	1	19	LEU
52	2	8	THR
53	3	28	VAL
53	3	34	LEU
53	3	38	SER
53	3	66	ILE
55	5	28	ARG
58	8	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	18	HIS
2	b	51	ASN

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Mol	Chain	Res	Type
2	b	168	HIS
2	b	227	GLN
3	c	25	ASN
3	c	69	HIS
3	c	100	GLN
3	c	102	ASN
3	c	176	HIS
4	d	136	GLN
5	e	89	HIS
5	e	132	ASN
6	f	3	HIS
6	f	52	ASN
6	f	94	HIS
9	i	31	ASN
9	i	110	GLN
11	k	118	HIS
14	n	35	ASN
14	n	49	GLN
14	n	60	GLN
14	n	66	GLN
15	o	50	HIS
15	o	80	GLN
16	p	79	ASN
19	s	56	GLN
20	t	48	GLN
20	t	52	ASN
21	u	64	ASN
26	z	91	ASN
26	z	160	GLN
26	z	252	GLN
26	z	274	ASN
26	z	302	HIS
26	z	356	ASN
26	z	365	HIS
29	C	86	ASN
29	C	117	GLN
30	D	36	GLN
31	E	92	HIS
31	E	115	GLN
31	E	195	GLN
32	F	52	ASN
32	F	127	ASN

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Mol	Chain	Res	Type
33	G	38	ASN
33	G	73	ASN
33	G	88	GLN
33	G	104	ASN
33	G	128	GLN
36	L	47	HIS
36	L	131	ASN
36	L	136	GLN
36	L	138	GLN
37	M	9	ASN
39	O	22	GLN
41	Q	29	HIS
41	Q	38	GLN
41	Q	61	GLN
41	Q	98	GLN
42	R	7	GLN
45	U	9	HIS
45	U	31	GLN
48	X	12	GLN
48	X	24	ASN
49	Y	46	HIS
49	Y	50	ASN
50	Z	36	HIS
51	1	39	GLN
53	3	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1527/1542 (99%)	220 (14%)	0
22	v	10/45 (22%)	1 (10%)	0
23	w	71/76 (93%)	16 (22%)	0
24	x	75/76 (98%)	11 (14%)	0
27	A	2897/2904 (99%)	395 (13%)	21 (0%)
28	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4699/4763 (98%)	660 (14%)	24 (0%)

All (660) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A

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Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	62	U
1	a	63	C
1	a	66	A
1	a	80	A
1	a	81	A
1	a	83	C
1	a	84	U
1	a	85	U
1	a	91	U
1	a	92	U
1	a	95	C
1	a	96	U
1	a	97	G
1	a	98	A
1	a	100	G
1	a	102	G
1	a	116	A
1	a	120	A
1	a	121	U
1	a	130	A
1	a	131	A
1	a	140	U
1	a	150	U
1	a	173	U
1	a	174	A
1	a	183	C
1	a	184	G
1	a	196	A
1	a	197	A
1	a	201	G
1	a	203	G
1	a	209	U

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Mol	Chain	Res	Type
1	a	210	C
1	a	211	G
1	a	219	U
1	a	220	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	321	A
1	a	328	C
1	a	338	A
1	a	339	C
1	a	341	C
1	a	346	G
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	356	A
1	a	367	U
1	a	372	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	415	A
1	a	421	U
1	a	424	G
1	a	429	U
1	a	430	A
1	a	456	A
1	a	464	U
1	a	465	A
1	a	467	U
1	a	478	A
1	a	480	U
1	a	484	G
1	a	486	U

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Mol	Chain	Res	Type
1	a	495	A
1	a	497	G
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	531	U
1	a	547	A
1	a	559	A
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	579	A
1	a	596	A
1	a	650	G
1	a	653	U
1	a	665	A
1	a	674	G
1	a	702	A
1	a	703	G
1	a	721	G
1	a	723	U
1	a	724	G
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	815	A
1	a	817	C
1	a	821	G
1	a	828	U
1	a	829	G
1	a	838	G
1	a	839	C
1	a	840	C
1	a	851	G
1	a	890	G
1	a	914	A
1	a	922	G
1	a	926	G

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Mol	Chain	Res	Type
1	a	934	C
1	a	935	A
1	a	936	C
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1000	A
1	a	1004	A
1	a	1008	U
1	a	1009	U
1	a	1020	G
1	a	1024	G
1	a	1025	U
1	a	1026	G
1	a	1027	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1036	A
1	a	1037	C
1	a	1038	C
1	a	1039	G
1	a	1043	G
1	a	1065	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1132	C
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1159	U
1	a	1169	A

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Mol	Chain	Res	Type
1	a	1184	G
1	a	1196	A
1	a	1197	A
1	a	1212	U
1	a	1213	A
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1258	G
1	a	1260	G
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1302	C
1	a	1317	C
1	a	1320	C
1	a	1331	G
1	a	1338	G
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1370	G
1	a	1378	C
1	a	1379	G
1	a	1397	C
1	a	1419	G
1	a	1428	A
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1448	C
1	a	1449	C
1	a	1450	U
1	a	1451	U
1	a	1452	C
1	a	1456	A
1	a	1457	G
1	a	1472	U
1	a	1487	G
1	a	1492	A
1	a	1493	A

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Mol	Chain	Res	Type
1	a	1494	G
1	a	1497	G
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
22	v	21	G
23	w	9	A
23	w	16	H2U
23	w	20	H2U
23	w	23	A
23	w	24	G
23	w	42	C
23	w	43	G
23	w	46	G7M
23	w	47	U
23	w	49	G
23	w	51	G
23	w	52	A
23	w	54	5MU
23	w	55	PSU
23	w	68	C
23	w	71	G
24	x	9	A
24	x	17	C
24	x	20	U
24	x	21	A
24	x	22	G
24	x	28	G
24	x	31	A
24	x	46	G7M
24	x	48	C
24	x	53	G
24	x	76	A
27	A	2	G
27	A	3	U
27	A	5	A
27	A	9	G
27	A	13	A

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Mol	Chain	Res	Type
27	A	15	G
27	A	34	U
27	A	58	G
27	A	60	G
27	A	71	A
27	A	74	A
27	A	75	G
27	A	100	U
27	A	101	A
27	A	118	A
27	A	119	A
27	A	120	U
27	A	131	A
27	A	139	U
27	A	143	C
27	A	145	C
27	A	146	A
27	A	147	C
27	A	148	U
27	A	163	C
27	A	164	C
27	A	181	A
27	A	196	A
27	A	216	A
27	A	222	A
27	A	233	A
27	A	248	G
27	A	267	C
27	A	269	C
27	A	271	G
27	A	272	A
27	A	275	C
27	A	279	A
27	A	280	U
27	A	281	C
27	A	282	A
27	A	287	G
27	A	295	G
27	A	311	A
27	A	329	G
27	A	330	A
27	A	353	C

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Mol	Chain	Res	Type
27	A	356	G
27	A	361	G
27	A	386	G
27	A	403	U
27	A	404	A
27	A	405	U
27	A	411	G
27	A	412	A
27	A	424	G
27	A	430	A
27	A	455	C
27	A	481	G
27	A	491	G
27	A	505	A
27	A	509	C
27	A	528	A
27	A	529	A
27	A	530	G
27	A	532	A
27	A	533	G
27	A	544	C
27	A	545	U
27	A	546	U
27	A	547	A
27	A	549	G
27	A	563	A
27	A	573	U
27	A	575	A
27	A	603	A
27	A	615	U
27	A	627	A
27	A	637	A
27	A	642	U
27	A	645	C
27	A	646	U
27	A	647	G
27	A	654	A
27	A	655	A
27	A	686	U
27	A	706	A
27	A	717	C
27	A	730	A

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Mol	Chain	Res	Type
27	A	747	5MU
27	A	764	A
27	A	765	C
27	A	775	G
27	A	776	G
27	A	782	A
27	A	784	G
27	A	785	G
27	A	789	A
27	A	805	G
27	A	812	C
27	A	827	U
27	A	828	U
27	A	845	A
27	A	846	U
27	A	859	G
27	A	877	A
27	A	891	G
27	A	895	U
27	A	896	A
27	A	897	C
27	A	900	A
27	A	910	A
27	A	912	C
27	A	914	G
27	A	915	C
27	A	927	A
27	A	931	U
27	A	946	C
27	A	961	C
27	A	974	G
27	A	983	A
27	A	996	A
27	A	1005	C
27	A	1012	U
27	A	1013	C
27	A	1026	G
27	A	1033	U
27	A	1038	G
27	A	1046	A
27	A	1047	G
27	A	1050	A

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Mol	Chain	Res	Type
27	A	1057	A
27	A	1059	G
27	A	1060	U
27	A	1061	U
27	A	1062	G
27	A	1064	C
27	A	1065	U
27	A	1069	A
27	A	1070	A
27	A	1071	G
27	A	1073	A
27	A	1074	G
27	A	1075	C
27	A	1076	C
27	A	1078	U
27	A	1079	C
27	A	1081	U
27	A	1082	U
27	A	1084	A
27	A	1085	A
27	A	1087	G
27	A	1088	A
27	A	1090	A
27	A	1094	U
27	A	1095	A
27	A	1101	U
27	A	1104	C
27	A	1111	A
27	A	1112	G
27	A	1118	C
27	A	1132	U
27	A	1134	A
27	A	1135	C
27	A	1142	A
27	A	1151	A
27	A	1212	G
27	A	1227	G
27	A	1253	A
27	A	1256	G
27	A	1271	G
27	A	1272	A
27	A	1300	G

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Mol	Chain	Res	Type
27	A	1301	A
27	A	1303	G
27	A	1352	U
27	A	1365	A
27	A	1379	U
27	A	1380	G
27	A	1383	A
27	A	1409	U
27	A	1414	C
27	A	1416	G
27	A	1417	C
27	A	1419	A
27	A	1420	A
27	A	1421	G
27	A	1428	C
27	A	1448	G
27	A	1449	G
27	A	1452	G
27	A	1453	A
27	A	1459	G
27	A	1460	U
27	A	1461	C
27	A	1482	G
27	A	1493	C
27	A	1494	A
27	A	1508	A
27	A	1509	A
27	A	1510	G
27	A	1515	A
27	A	1529	G
27	A	1535	A
27	A	1536	C
27	A	1537	G
27	A	1566	A
27	A	1569	A
27	A	1574	C
27	A	1575	C
27	A	1578	U
27	A	1580	A
27	A	1581	G
27	A	1583	A
27	A	1584	U

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Mol	Chain	Res	Type
27	A	1585	C
27	A	1608	A
27	A	1647	U
27	A	1648	U
27	A	1649	G
27	A	1674	G
27	A	1715	G
27	A	1724	G
27	A	1729	U
27	A	1730	C
27	A	1731	G
27	A	1738	G
27	A	1744	A
27	A	1764	C
27	A	1773	A
27	A	1776	G
27	A	1782	U
27	A	1784	A
27	A	1791	A
27	A	1800	C
27	A	1801	A
27	A	1808	A
27	A	1816	C
27	A	1848	A
27	A	1862	G
27	A	1871	A
27	A	1876	A
27	A	1906	G
27	A	1907	G
27	A	1919	A
27	A	1929	G
27	A	1930	G
27	A	1937	A
27	A	1938	A
27	A	1955	U
27	A	1965	C
27	A	1967	C
27	A	1970	A
27	A	1971	U
27	A	1972	G
27	A	1991	U
27	A	1993	U

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Mol	Chain	Res	Type
27	A	2023	C
27	A	2031	A
27	A	2033	A
27	A	2043	C
27	A	2051	A
27	A	2055	C
27	A	2056	G
27	A	2060	A
27	A	2061	G
27	A	2062	A
27	A	2069	G7M
27	A	2093	G
27	A	2110	G
27	A	2111	U
27	A	2112	G
27	A	2113	U
27	A	2115	G
27	A	2117	A
27	A	2118	U
27	A	2119	A
27	A	2120	G
27	A	2123	G
27	A	2124	G
27	A	2125	G
27	A	2128	G
27	A	2131	U
27	A	2132	U
27	A	2133	G
27	A	2135	A
27	A	2136	G
27	A	2145	C
27	A	2146	C
27	A	2147	A
27	A	2157	G
27	A	2159	G
27	A	2161	C
27	A	2165	C
27	A	2167	U
27	A	2171	A
27	A	2172	U
27	A	2173	A
27	A	2175	C

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Mol	Chain	Res	Type
27	A	2176	A
27	A	2178	C
27	A	2179	C
27	A	2180	U
27	A	2189	U
27	A	2190	G
27	A	2192	U
27	A	2198	A
27	A	2204	G
27	A	2212	A
27	A	2225	A
27	A	2238	G
27	A	2239	G
27	A	2268	A
27	A	2273	A
27	A	2283	C
27	A	2287	A
27	A	2298	A
27	A	2303	G
27	A	2304	G
27	A	2305	U
27	A	2308	G
27	A	2309	A
27	A	2312	U
27	A	2313	C
27	A	2322	A
27	A	2324	U
27	A	2325	G
27	A	2333	A
27	A	2335	A
27	A	2342	C
27	A	2347	C
27	A	2350	C
27	A	2361	G
27	A	2383	G
27	A	2385	C
27	A	2406	A
27	A	2422	C
27	A	2425	A
27	A	2428	G
27	A	2429	G
27	A	2430	A

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Mol	Chain	Res	Type
27	A	2431	U
27	A	2441	U
27	A	2448	A
27	A	2469	A
27	A	2470	G
27	A	2475	C
27	A	2476	A
27	A	2478	A
27	A	2490	G
27	A	2502	G
27	A	2505	G
27	A	2517	C
27	A	2518	A
27	A	2520	C
27	A	2529	G
27	A	2535	G
27	A	2547	A
27	A	2554	U
27	A	2566	A
27	A	2567	G
27	A	2572	A
27	A	2573	C
27	A	2602	A
27	A	2609	U
27	A	2613	U
27	A	2629	U
27	A	2670	A
27	A	2689	U
27	A	2690	U
27	A	2714	G
27	A	2716	C
27	A	2724	U
27	A	2726	A
27	A	2744	G
27	A	2748	A
27	A	2757	A
27	A	2758	A
27	A	2762	C
27	A	2765	A
27	A	2776	A
27	A	2778	A
27	A	2785	C

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Mol	Chain	Res	Type
27	A	2786	U
27	A	2790	U
27	A	2791	G
27	A	2800	A
27	A	2820	A
27	A	2821	A
27	A	2873	A
27	A	2884	U
27	A	2892	G
27	A	2899	A
27	A	2902	C
27	A	2903	U
28	B	4	C
28	B	8	C
28	B	9	G
28	B	10	G
28	B	13	G
28	B	24	G
28	B	25	U
28	B	35	C
28	B	51	G
28	B	56	G
28	B	65	U
28	B	67	G
28	B	89	U
28	B	90	C
28	B	108	A
28	B	109	A
28	B	115	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	142	A
27	A	527	C
27	A	529	A
27	A	764	A
27	A	784	G
27	A	1026	G
27	A	1046	A
27	A	1060	U
27	A	1075	C

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Mol	Chain	Res	Type
27	A	1084	A
27	A	1110	G
27	A	1647	U
27	A	2127	G
27	A	2178	C
27	A	2189	U
27	A	2191	A
27	A	2430	A
27	A	2489	U
27	A	2572	A
27	A	2756	U
27	A	2873	A
28	B	3	C
28	B	9	G
28	B	66	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

52 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	4D4	O	81	39	9,11,12	2.05	2 (22%)	7,13,15	1.76	2 (28%)
30	MEQ	D	150	30	8,9,10	0.91	0	5,10,12	1.30	1 (20%)
27	PSU	A	1917	27	18,21,22	1.62	4 (22%)	21,30,33	1.82	3 (14%)
1	2MG	a	1207	1	23,26,27	1.28	4 (17%)	33,38,41	2.05	7 (21%)
23	5MU	w	54	23	19,22,23	1.36	5 (26%)	27,32,35	2.16	7 (25%)
1	UR3	a	1498	1	19,22,23	0.87	0	26,32,35	1.92	4 (15%)
27	5MC	A	1962	60,27	19,22,23	1.47	3 (15%)	26,32,35	1.08	4 (15%)
27	PSU	A	2580	59,60,27	18,21,22	1.72	5 (27%)	21,30,33	1.87	5 (23%)
23	H2U	w	20	23	18,21,22	0.42	0	19,30,33	0.69	0
27	PSU	A	2457	27	18,21,22	1.57	4 (22%)	21,30,33	1.99	5 (23%)
12	D2T	l	89	12	8,9,10	1.35	0	6,11,13	1.76	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	2MG	A	1835	27	23,26,27	1.30	4 (17%)	33,38,41	2.08	7 (21%)
23	PSU	w	55	23	18,21,22	1.45	3 (16%)	21,30,33	2.02	4 (19%)
24	4SU	x	8	24	18,21,22	1.97	4 (22%)	25,30,33	1.99	5 (20%)
27	PSU	A	955	27	18,21,22	1.49	4 (22%)	21,30,33	2.05	4 (19%)
27	PSU	A	746	59,27	18,21,22	1.56	3 (16%)	21,30,33	2.06	5 (23%)
1	G7M	a	527	1	23,26,27	1.62	4 (17%)	34,39,42	1.63	4 (11%)
24	5MU	x	54	24	19,22,23	1.34	4 (21%)	27,32,35	2.07	6 (22%)
27	PSU	A	2504	59,60,27	18,21,22	1.41	3 (16%)	21,30,33	1.94	4 (19%)
24	PSU	x	55	24	18,21,22	1.39	3 (16%)	21,30,33	2.02	3 (14%)
39	MS6	O	82	39	5,7,8	0.59	0	2,7,9	1.13	0
24	PSU	x	32	24	18,21,22	1.41	3 (16%)	21,30,33	2.13	3 (14%)
1	2MG	a	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.39	10 (30%)
23	H2U	w	16	23	18,21,22	0.40	0	19,30,33	0.64	0
27	OMG	A	2251	60,27,24	23,26,27	1.31	4 (17%)	32,38,41	1.86	6 (18%)
27	PSU	A	2604	59,27	18,21,22	1.57	4 (22%)	21,30,33	1.72	3 (14%)
24	MIA	x	37	24	28,31,32	2.30	6 (21%)	38,44,47	2.56	13 (34%)
24	PSU	x	39	24	18,21,22	1.52	3 (16%)	21,30,33	2.07	5 (23%)
27	6MZ	A	1618	59,27	22,25,26	1.39	4 (18%)	29,36,39	2.45	12 (41%)
27	5MU	A	747	27	19,22,23	1.44	4 (21%)	27,32,35	1.72	5 (18%)
1	5MC	a	967	1	19,22,23	1.68	3 (15%)	26,32,35	1.14	4 (15%)
1	4OC	a	1402	59,1	20,23,24	0.76	0	25,32,35	1.00	2 (8%)
1	PSU	a	516	59,1	18,21,22	1.53	4 (22%)	21,30,33	1.85	3 (14%)
27	2MA	A	2503	59,60,27	22,25,26	1.44	5 (22%)	32,37,40	2.48	9 (28%)
27	6MZ	A	2030	27	22,25,26	1.47	5 (22%)	29,36,39	2.38	12 (41%)
27	1MG	A	745	59,27	23,26,27	1.21	4 (17%)	33,39,42	2.07	11 (33%)
27	2MG	A	2445	59,27	23,26,27	1.28	4 (17%)	33,38,41	2.09	8 (24%)
1	MA6	a	1518	1	23,26,27	1.54	5 (21%)	33,38,41	2.50	14 (42%)
27	PSU	A	2605	27	18,21,22	1.53	4 (22%)	21,30,33	1.99	4 (19%)
27	OMC	A	2498	59,27	19,22,23	0.70	0	25,31,34	0.83	0
27	OMU	A	2552	27	19,22,23	1.36	3 (15%)	25,31,34	1.75	5 (20%)
27	PSU	A	1911	27	18,21,22	1.42	3 (16%)	21,30,33	2.06	5 (23%)
27	H2U	A	2449	59,27	18,21,22	0.63	0	19,30,33	0.76	0
1	2MG	a	966	1	23,26,27	1.24	3 (13%)	33,38,41	2.25	7 (21%)
27	3TD	A	1915	27	19,22,23	6.74	11 (57%)	23,32,35	1.98	3 (13%)
1	5MC	a	1407	59,1	19,22,23	1.48	3 (15%)	26,32,35	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	a	1519	1	23,26,27	1.56	5 (21%)	33,38,41	2.45	12 (36%)
11	IAS	k	119	11	6,7,8	0.98	0	3,8,10	1.46	1 (33%)
27	G7M	A	2069	60,27	23,26,27	1.74	4 (17%)	34,39,42	1.44	3 (8%)
27	5MU	A	1939	60,27	19,22,23	1.45	4 (21%)	27,32,35	2.12	6 (22%)
24	G7M	x	46	24	23,26,27	1.58	4 (17%)	34,39,42	1.57	5 (14%)
23	G7M	w	46	23	23,26,27	2.37	5 (21%)	34,39,42	3.10	13 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	4D4	O	81	39	-	1/11/12/14	-
30	MEQ	D	150	30	-	4/8/9/11	-
27	PSU	A	1917	27	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
23	5MU	w	54	23	-	3/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
27	5MC	A	1962	60,27	-	0/7/25/26	0/2/2/2
27	PSU	A	2580	59,60,27	-	0/7/25/26	0/2/2/2
23	H2U	w	20	23	-	2/7/38/39	0/2/2/2
27	PSU	A	2457	27	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	4/7/12/14	-
27	2MG	A	1835	27	-	0/9/27/28	0/3/3/3
23	PSU	w	55	23	-	1/7/25/26	0/2/2/2
24	4SU	x	8	24	-	0/7/25/26	0/2/2/2
27	PSU	A	955	27	-	0/7/25/26	0/2/2/2
27	PSU	A	746	59,27	-	2/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
24	5MU	x	54	24	-	0/7/25/26	0/2/2/2
27	PSU	A	2504	59,60,27	-	1/7/25/26	0/2/2/2
24	PSU	x	55	24	-	0/7/25/26	0/2/2/2
39	MS6	O	82	39	-	1/4/6/8	-
24	PSU	x	32	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
23	H2U	w	16	23	-	3/7/38/39	0/2/2/2
27	OMG	A	2251	60,27,24	-	0/9/27/28	0/3/3/3
27	PSU	A	2604	59,27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MIA	x	37	24	-	2/15/33/34	0/3/3/3
24	PSU	x	39	24	-	0/7/25/26	0/2/2/2
27	6MZ	A	1618	59,27	-	0/9/27/28	0/3/3/3
27	5MU	A	747	27	-	1/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	59,1	-	0/9/29/30	0/2/2/2
1	PSU	a	516	59,1	-	0/7/25/26	0/2/2/2
27	2MA	A	2503	59,60,27	-	2/7/25/26	0/3/3/3
27	6MZ	A	2030	27	-	2/9/27/28	0/3/3/3
27	1MG	A	745	59,27	-	0/7/25/26	0/3/3/3
27	2MG	A	2445	59,27	-	0/9/27/28	0/3/3/3
1	MA6	a	1518	1	-	1/11/29/30	0/3/3/3
27	PSU	A	2605	27	-	0/7/25/26	0/2/2/2
27	OMC	A	2498	59,27	-	0/9/27/28	0/2/2/2
27	OMU	A	2552	27	-	0/9/27/28	0/2/2/2
27	PSU	A	1911	27	-	0/7/25/26	0/2/2/2
27	H2U	A	2449	59,27	-	0/7/38/39	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
27	3TD	A	1915	27	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	59,1	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	6/11/29/30	0/3/3/3
11	IAS	k	119	11	-	0/7/7/8	-
27	G7M	A	2069	60,27	-	2/7/25/26	0/3/3/3
27	5MU	A	1939	60,27	-	0/7/25/26	0/2/2/2
24	G7M	x	46	24	-	3/7/25/26	0/3/3/3
23	G7M	w	46	23	-	1/7/25/26	0/3/3/3

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1915	3TD	C2'-C1'	-15.41	1.32	1.53
27	A	1915	3TD	O4'-C1'	15.36	1.65	1.43
27	A	1915	3TD	C6-C5	12.64	1.49	1.35
27	A	1915	3TD	C2-N1	9.38	1.48	1.37
23	w	46	G7M	C8-N7	7.39	1.45	1.33
24	x	37	MIA	C2-S10	-7.13	1.69	1.75
24	x	37	MIA	C13-C14	6.99	1.53	1.32
27	A	1915	3TD	O4'-C4'	-6.38	1.30	1.45
1	a	967	5MC	C5-C4	6.14	1.48	1.44
27	A	2069	G7M	C5-N7	-5.76	1.32	1.39
27	A	1915	3TD	C6-N1	5.41	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1962	5MC	C5-C4	5.34	1.48	1.44
23	w	46	G7M	C5-N7	-5.23	1.33	1.39
24	x	46	G7M	C5-N7	-5.17	1.33	1.39
1	a	527	G7M	C5-N7	-5.13	1.33	1.39
1	a	1407	5MC	C5-C4	5.09	1.48	1.44
24	x	8	4SU	C4-S4	-5.02	1.59	1.68
39	O	81	4D4	CZ-NE	4.94	1.42	1.33
27	A	1915	3TD	C2-N3	4.85	1.48	1.38
24	x	8	4SU	C4-N3	-4.52	1.32	1.37
1	a	1518	MA6	C5-C4	4.28	1.46	1.39
1	a	1519	MA6	C5-C4	4.18	1.46	1.39
27	A	1618	6MZ	C5-C4	4.16	1.46	1.39
23	w	46	G7M	C8-N9	4.16	1.46	1.35
24	x	37	MIA	C5-C4	4.14	1.46	1.39
24	x	39	PSU	C4-N3	-3.88	1.31	1.38
27	A	2503	2MA	C5-C4	3.85	1.46	1.39
27	A	746	PSU	C6-C5	3.74	1.39	1.35
27	A	1915	3TD	O3'-C3'	-3.73	1.33	1.43
27	A	2552	OMU	C4-N3	-3.72	1.32	1.38
27	A	2030	6MZ	C5-C4	3.72	1.45	1.39
23	w	46	G7M	C5-C4	3.65	1.47	1.38
27	A	2580	PSU	C4-N3	-3.48	1.32	1.38
27	A	2069	G7M	C6-N1	-3.41	1.32	1.38
27	A	1939	5MU	C4-N3	-3.40	1.32	1.38
27	A	2580	PSU	C2-N3	-3.34	1.32	1.37
27	A	1917	PSU	C2-N3	-3.32	1.32	1.37
27	A	955	PSU	C4-N3	-3.31	1.32	1.38
27	A	2604	PSU	C4-N3	-3.30	1.32	1.38
27	A	746	PSU	C4-N3	-3.29	1.32	1.38
23	w	55	PSU	C6-C5	3.28	1.38	1.35
27	A	1911	PSU	C4-N3	-3.27	1.32	1.38
27	A	2580	PSU	C6-C5	3.27	1.38	1.35
1	a	516	PSU	C4-N3	-3.26	1.32	1.38
27	A	2251	OMG	C6-N1	-3.25	1.32	1.38
27	A	2605	PSU	C4-N3	-3.24	1.32	1.38
27	A	2604	PSU	C6-C5	3.21	1.38	1.35
27	A	747	5MU	C2-N3	-3.21	1.32	1.38
27	A	1917	PSU	C4-N3	-3.19	1.32	1.38
27	A	2504	PSU	C4-N3	-3.18	1.32	1.38
27	A	2604	PSU	C2-N3	-3.17	1.32	1.37
27	A	1915	3TD	O2-C2	-3.17	1.17	1.23
27	A	2457	PSU	C4-N3	-3.15	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2605	PSU	C6-C5	3.13	1.38	1.35
27	A	2504	PSU	C6-C5	3.11	1.38	1.35
27	A	2030	6MZ	C5-N7	-3.09	1.33	1.39
23	w	55	PSU	C4-N3	-3.08	1.33	1.38
27	A	747	5MU	C4-N3	-3.08	1.33	1.38
27	A	2069	G7M	C4-N9	-3.04	1.30	1.38
24	x	46	G7M	C5-C4	3.02	1.45	1.38
27	A	1917	PSU	C6-C5	3.00	1.38	1.35
24	x	55	PSU	C4-N3	-2.98	1.33	1.38
27	A	1835	2MG	C6-N1	-2.96	1.33	1.38
27	A	2030	6MZ	C4-N9	-2.95	1.31	1.37
24	x	55	PSU	C6-C5	2.94	1.38	1.35
1	a	1519	MA6	C5-C6	2.94	1.48	1.41
1	a	966	2MG	C5-C4	2.94	1.46	1.38
27	A	1939	5MU	C2-N3	-2.93	1.32	1.38
24	x	32	PSU	C4-N3	-2.92	1.33	1.38
1	a	1519	MA6	C5-N7	-2.91	1.33	1.39
1	a	1207	2MG	C6-N1	-2.91	1.33	1.38
27	A	2457	PSU	C6-C5	2.91	1.38	1.35
24	x	54	5MU	C4-N3	-2.90	1.33	1.38
27	A	745	1MG	C5-N7	-2.90	1.33	1.39
1	a	1516	2MG	C6-N1	-2.89	1.33	1.38
1	a	516	PSU	C6-C5	2.89	1.38	1.35
24	x	32	PSU	C6-C5	2.87	1.38	1.35
27	A	2457	PSU	C2-N1	-2.87	1.32	1.36
24	x	8	4SU	C5-C4	-2.86	1.39	1.42
27	A	2552	OMU	C2-N3	-2.86	1.33	1.38
1	a	966	2MG	C6-N1	-2.85	1.33	1.38
1	a	1518	MA6	C5-C6	2.84	1.48	1.41
27	A	2251	OMG	C5-C4	2.82	1.46	1.38
27	A	2503	2MA	C5-N7	-2.82	1.33	1.39
1	a	527	G7M	C6-N1	-2.82	1.33	1.38
27	A	745	1MG	C5-C4	2.80	1.46	1.38
27	A	955	PSU	C6-C5	2.80	1.38	1.35
27	A	2605	PSU	C2-N3	-2.79	1.32	1.37
1	a	527	G7M	C4-N9	-2.78	1.31	1.38
39	O	81	4D4	CZ-NH1	2.77	1.44	1.34
24	x	8	4SU	C2-N3	-2.76	1.33	1.38
24	x	37	MIA	C5-N7	-2.75	1.34	1.39
23	w	54	5MU	C4-N3	-2.74	1.33	1.38
27	A	2580	PSU	C2-N1	-2.73	1.33	1.36
1	a	967	5MC	C6-C5	2.72	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1618	6MZ	C5-N7	-2.72	1.34	1.39
27	A	2457	PSU	C2-N3	-2.72	1.33	1.37
27	A	1835	2MG	C5-C4	2.71	1.46	1.38
1	a	516	PSU	C2-N3	-2.71	1.33	1.37
27	A	2445	2MG	C5-N7	-2.69	1.33	1.39
27	A	747	5MU	C6-C5	2.67	1.39	1.34
1	a	1518	MA6	C5-N7	-2.66	1.34	1.39
27	A	1911	PSU	C6-C5	2.64	1.38	1.35
1	a	527	G7M	C5-C4	2.62	1.44	1.38
1	a	1207	2MG	C5-C4	2.62	1.45	1.38
27	A	2251	OMG	C5-N7	-2.61	1.33	1.39
27	A	2445	2MG	C5-C4	2.61	1.45	1.38
27	A	2445	2MG	C6-N1	-2.58	1.34	1.38
24	x	39	PSU	C2-N3	-2.58	1.33	1.37
1	a	1516	2MG	C5-C4	2.57	1.45	1.38
1	a	1207	2MG	C5-N7	-2.57	1.33	1.39
27	A	746	PSU	C2-N3	-2.56	1.33	1.37
27	A	1835	2MG	C5-N7	-2.56	1.33	1.39
24	x	46	G7M	C6-N1	-2.56	1.34	1.38
27	A	1939	5MU	C6-C5	2.56	1.38	1.34
24	x	39	PSU	C6-C5	2.56	1.38	1.35
27	A	1911	PSU	C2-N3	-2.55	1.33	1.37
1	a	1407	5MC	C6-N1	-2.55	1.33	1.38
27	A	1915	3TD	O4-C4	-2.55	1.17	1.23
1	a	1516	2MG	C5-N7	-2.54	1.34	1.39
24	x	54	5MU	C2-N3	-2.54	1.33	1.38
27	A	2069	G7M	C5-C4	2.52	1.44	1.38
27	A	1915	3TD	C4-N3	2.51	1.45	1.40
1	a	1407	5MC	C6-C5	2.51	1.38	1.34
27	A	745	1MG	C4-N9	-2.49	1.31	1.38
27	A	1917	PSU	C2-N1	-2.49	1.33	1.36
1	a	1518	MA6	C4-N9	-2.48	1.32	1.37
27	A	1835	2MG	C4-N9	-2.47	1.31	1.38
27	A	955	PSU	C2-N3	-2.46	1.33	1.37
1	a	1519	MA6	C4-N9	-2.45	1.32	1.37
24	x	54	5MU	C6-C5	2.43	1.38	1.34
27	A	2251	OMG	C4-N9	-2.43	1.31	1.38
27	A	745	1MG	C2-N1	2.43	1.41	1.37
24	x	32	PSU	C2-N3	-2.42	1.33	1.37
1	a	1207	2MG	C4-N9	-2.41	1.31	1.38
23	w	54	5MU	C2-N3	-2.41	1.33	1.38
23	w	54	5MU	C2-N1	2.40	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2503	2MA	C5-C6	2.40	1.47	1.41
23	w	55	PSU	C2-N3	-2.40	1.33	1.37
27	A	955	PSU	C2-N1	-2.38	1.33	1.36
1	a	516	PSU	C2-N1	-2.35	1.33	1.36
27	A	1618	6MZ	C5-C6	2.34	1.47	1.41
24	x	46	G7M	C4-N9	-2.34	1.32	1.38
27	A	1962	5MC	C6-N1	-2.33	1.34	1.38
27	A	1939	5MU	C6-N1	-2.32	1.34	1.38
1	a	966	2MG	C5-N7	-2.32	1.34	1.39
1	a	967	5MC	C6-N1	-2.32	1.34	1.38
27	A	2604	PSU	C2-N1	-2.29	1.33	1.36
27	A	2445	2MG	C4-N9	-2.29	1.32	1.38
27	A	2030	6MZ	C8-N9	-2.27	1.33	1.37
23	w	54	5MU	C6-C5	2.27	1.38	1.34
27	A	747	5MU	C6-N1	-2.26	1.34	1.38
23	w	46	G7M	C6-N1	-2.26	1.34	1.38
24	x	37	MIA	C5-C6	2.24	1.47	1.41
27	A	2552	OMU	C5-C4	-2.21	1.38	1.43
27	A	2580	PSU	O4'-C1'	-2.20	1.40	1.43
27	A	2503	2MA	C4-N9	-2.17	1.33	1.37
27	A	1618	6MZ	C4-N9	-2.16	1.33	1.37
1	a	1519	MA6	C8-N9	-2.16	1.33	1.37
1	a	1516	2MG	C4-N9	-2.15	1.32	1.38
27	A	2503	2MA	C8-N9	-2.15	1.33	1.37
24	x	54	5MU	C6-N1	-2.14	1.34	1.38
27	A	2504	PSU	C2-N3	-2.11	1.34	1.37
27	A	2030	6MZ	C5-C6	2.10	1.47	1.41
24	x	37	MIA	C4-N9	-2.10	1.33	1.37
24	x	55	PSU	C2-N3	-2.09	1.34	1.37
27	A	1962	5MC	C6-C5	2.09	1.38	1.34
23	w	54	5MU	C6-N1	-2.02	1.34	1.38
27	A	2605	PSU	C2-N1	-2.02	1.34	1.36
1	a	1518	MA6	C8-N9	-2.01	1.34	1.37

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2503	2MA	C5-C4-N3	-8.34	118.39	127.18
23	w	46	G7M	CN7-N7-C8	-7.87	112.88	124.79
1	a	1498	UR3	C4-N3-C2	-7.76	118.33	124.58
24	x	37	MIA	C5-C4-N3	-7.71	119.06	127.18
1	a	1516	2MG	C2-N3-C4	7.63	121.55	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C2-N3-C4	7.54	121.43	112.00
27	A	2445	2MG	C2-N3-C4	6.92	120.66	112.00
27	A	1835	2MG	C2-N3-C4	6.90	120.63	112.00
27	A	2503	2MA	N3-C4-N9	6.87	135.71	126.99
27	A	2605	PSU	N1-C2-N3	6.75	122.29	115.17
1	a	1207	2MG	C2-N3-C4	6.72	120.41	112.00
24	x	37	MIA	N3-C4-N9	6.71	135.51	126.99
27	A	746	PSU	N1-C2-N3	6.64	122.17	115.17
23	w	46	G7M	N9-C8-N7	-6.52	96.64	112.48
24	x	32	PSU	N1-C2-N3	6.49	122.01	115.17
24	x	37	MIA	C12-C13-C14	-6.47	115.40	127.01
27	A	1911	PSU	N1-C2-N3	6.46	121.98	115.17
24	x	39	PSU	N1-C2-N3	6.44	121.96	115.17
23	w	55	PSU	N1-C2-N3	6.44	121.96	115.17
24	x	55	PSU	N1-C2-N3	6.42	121.94	115.17
23	w	46	G7M	C8-N7-C5	6.36	115.74	107.78
1	a	966	2MG	C5-C4-N3	-6.32	118.33	128.39
27	A	955	PSU	N1-C2-N3	6.30	121.82	115.17
27	A	1917	PSU	N1-C2-N3	6.11	121.61	115.17
23	w	46	G7M	N9-C4-N3	6.10	138.16	125.95
27	A	1618	6MZ	C5-C4-N3	-6.08	118.34	126.72
1	a	516	PSU	N1-C2-N3	6.08	121.58	115.17
27	A	2457	PSU	N1-C2-N3	6.03	121.53	115.17
1	a	1516	2MG	C5-C4-N3	-5.89	119.02	128.39
27	A	1915	3TD	N1-C2-N3	5.85	120.38	116.13
1	a	1519	MA6	C5-C4-N3	-5.78	118.76	126.72
27	A	2580	PSU	N1-C2-N3	5.72	121.20	115.17
27	A	2604	PSU	N1-C2-N3	5.63	121.11	115.17
24	x	8	4SU	C4-N3-C2	-5.60	121.94	127.31
23	w	46	G7M	C5-C4-N3	-5.56	117.64	128.15
27	A	2504	PSU	N1-C2-N3	5.54	121.01	115.17
27	A	2251	OMG	C5-C4-N3	-5.42	119.77	128.39
23	w	54	5MU	N3-C2-N1	5.40	121.92	114.89
27	A	1835	2MG	C5-C4-N3	-5.39	119.81	128.39
1	a	1518	MA6	C5-C4-N3	-5.36	119.34	126.72
27	A	1939	5MU	N3-C2-N1	5.32	121.81	114.89
27	A	1618	6MZ	N3-C4-N9	5.28	136.14	127.17
1	a	1207	2MG	C5-C4-N3	-5.22	120.09	128.39
27	A	1939	5MU	C4-N3-C2	-5.16	120.58	127.34
24	x	8	4SU	C5-C4-N3	5.11	119.50	114.75
27	A	745	1MG	C5-C4-N3	-5.10	120.27	128.39
24	x	54	5MU	N3-C2-N1	5.02	121.42	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	54	5MU	C4-N3-C2	-5.01	120.77	127.34
27	A	2445	2MG	C5-C4-N3	-5.00	120.43	128.39
27	A	2030	6MZ	C6-C5-N7	4.93	137.81	132.43
23	w	54	5MU	C4-N3-C2	-4.93	120.88	127.34
1	a	1519	MA6	C4-C5-N7	-4.93	104.95	110.58
1	a	966	2MG	N9-C4-N3	4.92	135.80	125.95
24	x	46	G7M	C5-C4-N3	-4.88	118.93	128.15
1	a	1518	MA6	C2-N1-C6	4.85	123.68	111.83
27	A	1939	5MU	C5-C4-N3	4.85	119.54	115.32
27	A	1915	3TD	C4-N3-C2	-4.75	119.58	124.61
1	a	527	G7M	C5-C4-N3	-4.73	119.21	128.15
24	x	46	G7M	N9-C4-N3	4.73	135.40	125.95
1	a	527	G7M	C2-N3-C4	4.66	120.33	112.30
27	A	745	1MG	N2-C2-N1	4.62	122.50	118.79
27	A	2030	6MZ	C5-C4-N3	-4.60	120.38	126.72
27	A	2251	OMG	C2-N3-C4	4.60	120.22	112.30
24	x	37	MIA	C15-C14-C13	-4.56	108.98	122.66
1	a	1518	MA6	N1-C6-N6	4.54	122.39	116.86
27	A	747	5MU	N3-C2-N1	4.52	120.78	114.89
24	x	54	5MU	C5-C4-N3	4.50	119.24	115.32
24	x	32	PSU	C4-N3-C2	-4.49	120.18	126.37
27	A	2552	OMU	C4-N3-C2	-4.49	121.04	126.61
23	w	46	G7M	C2-N3-C4	4.47	120.00	112.30
1	a	1519	MA6	C10-N6-C6	-4.47	109.16	120.52
1	a	1516	2MG	N9-C4-N3	4.46	134.87	125.95
27	A	2552	OMU	N3-C2-N1	4.42	120.64	114.89
1	a	1518	MA6	C4-C5-N7	-4.41	105.54	110.58
1	a	1519	MA6	C2-N1-C6	4.41	122.59	111.83
27	A	745	1MG	C2-N3-C4	4.39	121.84	111.98
24	x	39	PSU	C4-N3-C2	-4.35	120.37	126.37
23	w	46	G7M	O4'-C1'-N9	4.31	118.13	108.36
24	x	8	4SU	N3-C2-N1	4.30	120.49	114.89
24	x	46	G7M	C2-N3-C4	4.28	119.68	112.30
24	x	54	5MU	O4-C4-C5	-4.23	120.08	124.92
27	A	2030	6MZ	N1-C2-N3	-4.23	122.18	128.58
27	A	1911	PSU	C4-N3-C2	-4.21	120.57	126.37
1	a	1516	2MG	N1-C2-N2	4.15	120.80	116.56
1	a	1518	MA6	N3-C4-N9	4.12	134.18	127.17
27	A	2251	OMG	N9-C4-N3	4.12	134.19	125.95
27	A	955	PSU	O2-C2-N1	-4.10	118.56	122.79
27	A	1618	6MZ	C2-N3-C4	4.09	121.83	111.83
27	A	2069	G7M	C5-C4-N3	-4.09	120.43	128.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1207	2MG	N9-C4-N3	4.05	134.04	125.95
23	w	54	5MU	O4-C4-C5	-4.03	120.31	124.92
27	A	746	PSU	C4-N3-C2	-3.98	120.89	126.37
1	a	1519	MA6	N3-C4-N9	3.98	133.94	127.17
23	w	54	5MU	C5-C4-N3	3.96	118.77	115.32
27	A	1939	5MU	O4-C4-C5	-3.96	120.39	124.92
1	a	527	G7M	N9-C4-N3	3.94	133.83	125.95
1	a	1518	MA6	N1-C2-N3	-3.93	122.63	128.58
27	A	955	PSU	C4-N3-C2	-3.93	120.96	126.37
27	A	2504	PSU	C4-N3-C2	-3.93	120.96	126.37
1	a	1519	MA6	C2-N3-C4	3.92	121.41	111.83
27	A	2030	6MZ	N3-C4-N9	3.92	133.84	127.17
27	A	745	1MG	N9-C4-N3	3.92	133.79	125.95
27	A	2030	6MZ	C4-N9-C8	3.90	109.83	105.74
24	x	55	PSU	C4-N3-C2	-3.90	121.00	126.37
23	w	46	G7M	C8-N9-C4	3.88	116.69	107.09
27	A	2445	2MG	N9-C4-N3	3.86	133.68	125.95
23	w	55	PSU	C4-N3-C2	-3.85	121.07	126.37
27	A	1939	5MU	C5-C6-N1	-3.85	119.14	123.31
27	A	2069	G7M	N9-C4-N3	3.84	133.63	125.95
27	A	2445	2MG	C6-C5-N7	3.83	137.26	130.29
27	A	2457	PSU	O2-C2-N1	-3.83	118.84	122.79
27	A	1618	6MZ	N1-C2-N3	-3.81	122.81	128.58
1	a	1518	MA6	C2-N3-C4	3.77	121.04	111.83
27	A	1835	2MG	C6-C5-N7	3.74	137.10	130.29
27	A	2552	OMU	C5-C4-N3	3.73	120.02	114.80
27	A	747	5MU	C4-N3-C2	-3.73	122.45	127.34
27	A	2457	PSU	C4-N3-C2	-3.71	121.25	126.37
23	w	46	G7M	CN7-N7-C5	3.68	131.39	126.80
1	a	1516	2MG	C6-C5-N7	3.66	136.95	130.29
27	A	1835	2MG	N9-C4-N3	3.66	133.26	125.95
27	A	2503	2MA	C4-C5-N7	-3.65	106.41	110.58
27	A	1915	3TD	C3'-C2'-C1'	3.65	105.99	101.69
27	A	747	5MU	O4-C4-C5	-3.63	120.77	124.92
27	A	2251	OMG	C6-C5-N7	3.62	136.88	130.29
1	a	1498	UR3	C5-C4-N3	3.62	119.81	115.04
24	x	54	5MU	C5-C6-N1	-3.61	119.39	123.31
27	A	2030	6MZ	C2-N3-C4	3.60	120.62	111.83
1	a	1519	MA6	C5-N7-C8	3.58	109.08	103.45
24	x	55	PSU	O2-C2-N1	-3.58	119.10	122.79
27	A	2503	2MA	C4-N9-C8	3.54	109.46	105.74
27	A	2069	G7M	C2-N3-C4	3.52	118.36	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2030	6MZ	C4-C5-N7	-3.48	106.60	110.58
27	A	2503	2MA	N6-C6-N1	3.47	121.71	117.03
1	a	1207	2MG	C6-C5-N7	3.45	136.57	130.29
27	A	2605	PSU	C4-N3-C2	-3.44	121.62	126.37
1	a	1519	MA6	N1-C2-N3	-3.42	123.40	128.58
1	a	1518	MA6	C5-N7-C8	3.40	108.80	103.45
24	x	37	MIA	C16-C14-C13	-3.39	112.49	122.66
1	a	1518	MA6	C4-N9-C8	3.39	109.30	105.74
24	x	32	PSU	O2-C2-N1	-3.37	119.31	122.79
27	A	1618	6MZ	C4-N9-C8	3.33	109.24	105.74
27	A	747	5MU	C5-C4-N3	3.31	118.20	115.32
39	O	81	4D4	O-C-CA	-3.31	116.26	124.77
27	A	2030	6MZ	C9-N6-C6	-3.29	119.80	122.85
27	A	747	5MU	C5-C6-N1	-3.28	119.75	123.31
27	A	2580	PSU	C4-N3-C2	-3.26	121.88	126.37
27	A	1618	6MZ	C6-C5-N7	3.26	135.98	132.43
27	A	1618	6MZ	O2'-C2'-C3'	3.21	122.12	111.82
24	x	37	MIA	C2-N3-C4	3.21	120.69	112.29
1	a	967	5MC	C5-C4-N3	-3.19	118.48	121.75
27	A	2504	PSU	C6-C5-C4	-3.17	116.04	118.17
27	A	1618	6MZ	C4-C5-N7	-3.15	106.98	110.58
23	w	46	G7M	C1'-N9-C8	-3.15	116.11	126.74
27	A	2503	2MA	C5-N7-C8	3.11	108.34	103.45
1	a	966	2MG	C6-C5-N7	3.10	135.94	130.29
23	w	46	G7M	C2'-C1'-N9	3.06	121.78	113.25
1	a	1407	5MC	C5-C6-N1	-3.01	120.04	123.31
27	A	2504	PSU	O2-C2-N1	-3.01	119.69	122.79
27	A	746	PSU	C6-C5-C4	-3.00	116.15	118.17
1	a	516	PSU	C4-N3-C2	-2.99	122.25	126.37
24	x	37	MIA	C4-N9-C8	2.97	108.86	105.74
27	A	1911	PSU	O2-C2-N1	-2.96	119.73	122.79
27	A	745	1MG	C6-C5-N7	2.94	135.89	129.36
27	A	2030	6MZ	N9-C8-N7	-2.93	109.78	113.94
1	a	1518	MA6	C9-N6-C6	-2.92	113.08	120.52
27	A	2030	6MZ	C5-N7-C8	2.90	108.00	103.45
23	w	54	5MU	C5-C6-N1	-2.89	120.18	123.31
27	A	1618	6MZ	O2'-C2'-C1'	2.88	120.03	110.10
24	x	39	PSU	O2-C2-N1	-2.87	119.83	122.79
27	A	1917	PSU	C4-N3-C2	-2.86	122.43	126.37
27	A	1917	PSU	O2-C2-N3	-2.86	116.78	121.86
1	a	1518	MA6	N9-C8-N7	-2.86	109.89	113.94
23	w	46	G7M	O6-C6-C5	-2.85	121.66	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2503	2MA	N9-C8-N7	-2.85	109.90	113.94
1	a	967	5MC	C5-C6-N1	-2.83	120.24	123.31
27	A	2604	PSU	O2-C2-N3	-2.83	116.84	121.86
1	a	1519	MA6	C10-N6-C9	-2.82	107.11	116.18
23	w	55	PSU	O2-C2-N1	-2.81	119.89	122.79
27	A	1835	2MG	C4-C5-N7	-2.77	106.29	110.67
27	A	1618	6MZ	C5-N7-C8	2.75	107.77	103.45
1	a	1407	5MC	C5-C4-N3	-2.75	118.94	121.75
27	A	1835	2MG	N1-C2-N2	2.73	119.35	116.56
23	w	54	5MU	C1'-N1-C2	2.73	122.49	117.59
1	a	516	PSU	O2-C2-N1	-2.72	119.99	122.79
27	A	2580	PSU	C6-C5-C4	-2.71	116.34	118.17
27	A	1962	5MC	C5-C6-N1	-2.71	120.37	123.31
24	x	37	MIA	C4-C5-N7	-2.70	107.50	110.58
27	A	2445	2MG	C4-C5-N7	-2.65	106.47	110.67
1	a	1519	MA6	N9-C8-N7	-2.62	110.22	113.94
1	a	1516	2MG	C4-C5-N7	-2.61	106.53	110.67
27	A	745	1MG	C4-C5-N7	-2.61	106.54	110.67
27	A	745	1MG	C2-N1-C6	-2.59	118.82	120.99
23	w	54	5MU	O2-C2-N3	-2.58	116.72	121.49
1	a	1516	2MG	N2-C2-N3	-2.57	117.24	120.51
1	a	1519	MA6	C6-C5-N7	2.57	137.53	133.43
1	a	1519	MA6	C4-N9-C8	2.56	108.43	105.74
27	A	745	1MG	CM1-N1-C2	2.55	123.34	120.70
27	A	2605	PSU	O2-C2-N3	-2.53	117.36	121.86
24	x	54	5MU	O2-C2-N1	-2.52	119.51	122.80
24	x	37	MIA	C2-N1-C6	2.52	122.32	117.54
27	A	746	PSU	O2-C2-N3	-2.50	117.41	121.86
24	x	39	PSU	C5-C6-N1	-2.49	118.68	122.14
24	x	37	MIA	N6-C6-N1	2.48	121.65	118.33
27	A	2030	6MZ	C2-N1-C6	2.46	123.39	115.24
1	a	966	2MG	O6-C6-C5	-2.44	120.09	126.53
27	A	1962	5MC	CM5-C5-C6	-2.44	119.55	122.85
27	A	1618	6MZ	N9-C8-N7	-2.43	110.49	113.94
11	k	119	IAS	OD1-CG-CB	-2.43	118.31	125.38
27	A	2251	OMG	C4-C5-N7	-2.41	106.84	110.67
24	x	37	MIA	N3-C2-N1	-2.39	122.63	127.00
27	A	2604	PSU	C4-N3-C2	-2.39	123.08	126.37
1	a	1518	MA6	C5-C6-N6	-2.38	121.57	125.33
27	A	2605	PSU	O2-C2-N1	-2.36	120.35	122.79
24	x	37	MIA	C6-C5-N7	2.35	134.99	132.43
39	O	81	4D4	NE-CZ-NH2	2.35	124.70	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C4-C5-N7	-2.34	106.97	110.67
24	x	8	4SU	O2-C2-N1	-2.31	119.78	122.80
1	a	1518	MA6	C6-C5-N7	2.31	137.12	133.43
27	A	746	PSU	O2-C2-N1	-2.30	120.41	122.79
24	x	37	MIA	C5-N7-C8	2.30	107.07	103.45
1	a	1402	4OC	C6-C5-C4	2.30	119.77	117.00
27	A	2503	2MA	C6-C5-N7	2.30	136.52	132.09
27	A	2580	PSU	O2-C2-N1	-2.30	120.42	122.79
24	x	8	4SU	C5-C4-S4	-2.30	121.68	124.31
27	A	2445	2MG	C8-N7-C5	2.29	108.34	104.26
1	a	1207	2MG	O6-C6-C5	-2.28	120.50	126.53
1	a	1207	2MG	C4-C5-N7	-2.26	107.09	110.67
1	a	1518	MA6	C10-N6-C6	-2.25	114.79	120.52
27	A	2580	PSU	O4'-C1'-C2'	2.25	108.26	105.15
27	A	745	1MG	N2-C2-N3	-2.25	114.63	119.75
12	l	89	D2T	O-C-CA	-2.24	119.00	124.77
27	A	2552	OMU	O2-C2-N1	-2.21	119.92	122.80
1	a	1407	5MC	O2-C2-N3	-2.20	118.86	122.33
27	A	2503	2MA	C2-N1-C6	2.20	121.48	118.10
1	a	1402	4OC	O2-C2-N3	-2.18	118.89	122.33
27	A	2445	2MG	N1-C2-N2	2.18	118.78	116.56
1	a	967	5MC	O2-C2-N3	-2.18	118.90	122.33
27	A	2030	6MZ	C4-N9-C1'	-2.16	121.59	126.63
1	a	967	5MC	CM5-C5-C6	-2.16	119.93	122.85
30	D	150	MEQ	CG-CD-NE2	2.15	119.40	116.39
27	A	2552	OMU	O4-C4-C5	-2.13	121.48	125.16
27	A	1962	5MC	C5-C4-N3	-2.13	119.57	121.75
1	a	1516	2MG	C8-N7-C5	2.12	108.04	104.26
27	A	2457	PSU	C6-C5-C4	-2.12	116.74	118.17
24	x	46	G7M	O6-C6-C5	-2.12	123.29	128.01
27	A	745	1MG	C6-C5-C4	-2.12	117.57	119.97
27	A	745	1MG	C8-N7-C5	2.11	108.03	104.26
27	A	955	PSU	C5-C6-N1	-2.10	119.22	122.14
27	A	1939	5MU	O2-C2-N1	-2.10	120.07	122.80
23	w	55	PSU	O2-C2-N3	-2.09	118.15	121.86
1	a	1516	2MG	C5-C6-N1	2.09	118.57	113.25
1	a	966	2MG	C5-C6-N1	2.09	118.57	113.25
27	A	2445	2MG	O6-C6-C5	-2.08	121.03	126.53
1	a	1498	UR3	C3U-N3-C2	2.08	120.95	117.33
27	A	1911	PSU	C5-C6-N1	-2.07	119.26	122.14
1	a	1516	2MG	O6-C6-C5	-2.07	121.08	126.53
12	l	89	D2T	CB-CA-N	2.06	113.27	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	G7M	C1'-N9-C4	-2.06	120.41	126.49
27	A	2251	OMG	O6-C6-C5	-2.05	121.11	126.53
24	x	39	PSU	O2-C2-N3	-2.05	118.22	121.86
27	A	1618	6MZ	C2-N1-C6	2.05	122.04	115.24
1	a	1498	UR3	C3U-N3-C4	2.05	120.71	117.87
27	A	1835	2MG	O6-C6-C5	-2.04	121.14	126.53
1	a	1207	2MG	N1-C2-N2	2.03	118.64	116.56
23	w	46	G7M	C5-C6-N1	2.03	116.04	111.84
27	A	1962	5MC	O2-C2-N3	-2.02	119.15	122.33
27	A	1911	PSU	O2-C2-N3	-2.01	118.29	121.86
27	A	2457	PSU	O4'-C1'-C2'	2.01	107.93	105.15
24	x	46	G7M	C5-C6-N1	2.00	115.98	111.84

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
24	x	37	MIA	N6-C12-C13-C14
24	x	37	MIA	C12-C13-C14-C16
24	x	46	G7M	C4'-C5'-O5'-P
24	x	46	G7M	O4'-C4'-C5'-O5'
30	D	150	MEQ	C-CA-CB-CG
30	D	150	MEQ	O-C-CA-CB
1	a	527	G7M	C3'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
24	x	46	G7M	C3'-C4'-C5'-O5'
30	D	150	MEQ	OE1-CD-CG-CB
30	D	150	MEQ	NE2-CD-CG-CB
1	a	1519	MA6	C3'-C4'-C5'-O5'
23	w	16	H2U	C3'-C4'-C5'-O5'
23	w	16	H2U	O4'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
27	A	2030	6MZ	O4'-C4'-C5'-O5'
27	A	2030	6MZ	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
23	w	16	H2U	C4'-C5'-O5'-P
27	A	747	5MU	C3'-C4'-C5'-O5'
23	w	46	G7M	C4'-C5'-O5'-P
23	w	55	PSU	O4'-C1'-C5-C4
23	w	54	5MU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
23	w	54	5MU	C2'-C1'-N1-C6
27	A	2069	G7M	C4'-C5'-O5'-P
23	w	20	H2U	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C10
23	w	54	5MU	C2'-C1'-N1-C2
27	A	2503	2MA	C4'-C5'-O5'-P
27	A	2504	PSU	O4'-C4'-C5'-O5'
12	l	89	D2T	SB-CB-CG-OD2
27	A	746	PSU	O4'-C1'-C5-C6
39	O	82	MS6	CB-CG-SD-CE
27	A	2069	G7M	O4'-C4'-C5'-O5'
12	l	89	D2T	CA-CB-CG-OD1
12	l	89	D2T	CA-CB-CG-OD2
12	l	89	D2T	CG-CB-SB-CB1
27	A	746	PSU	C2'-C1'-C5-C6
39	O	81	4D4	O-C-CA-CB
1	a	1519	MA6	C4'-C5'-O5'-P
23	w	20	H2U	C4'-C5'-O5'-P
27	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1917	PSU	1	0
1	a	1207	2MG	1	0
23	w	54	5MU	1	0
23	w	55	PSU	1	0
23	w	16	H2U	1	0
27	A	2251	OMG	1	0
27	A	2604	PSU	1	0
27	A	2030	6MZ	2	0
1	a	1518	MA6	1	0
27	A	1915	3TD	1	0
1	a	1407	5MC	1	0
1	a	1519	MA6	1	0
27	A	1939	5MU	1	0
24	x	46	G7M	2	0
23	w	46	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 986 ligands modelled in this entry, 984 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	MQH	z	402	-	56,61,61	2.57	15 (26%)	77,89,89	2.43	18 (23%)
61	GDP	z	401	-	29,30,30	1.21	4 (13%)	45,47,47	1.74	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	MQH	z	402	-	-	19/81/96/96	0/3/4/4
61	GDP	z	401	-	-	3/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	z	402	MQH	C23-N24	7.89	1.51	1.34
62	z	402	MQH	C02-N03	7.65	1.50	1.34
62	z	402	MQH	C12-N13	7.60	1.50	1.34
62	z	402	MQH	C47-N46	7.41	1.49	1.34
62	z	402	MQH	C54-N53	5.51	1.51	1.35
62	z	402	MQH	C09-N10	3.38	1.35	1.28
62	z	402	MQH	O28-C27	3.15	1.42	1.33
62	z	402	MQH	C33-C34	2.93	1.41	1.34
61	z	401	GDP	C5-C4	2.89	1.46	1.38
62	z	402	MQH	O58-C47	-2.80	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	401	GDP	C6-N1	-2.69	1.33	1.38
62	z	402	MQH	O01-C02	-2.67	1.18	1.23
62	z	402	MQH	O36-C23	-2.54	1.18	1.23
61	z	401	GDP	C5-N7	-2.40	1.34	1.39
61	z	401	GDP	C4-N9	-2.33	1.32	1.38
62	z	402	MQH	C41-C38	2.20	1.58	1.53
62	z	402	MQH	O37-C12	-2.13	1.19	1.23
62	z	402	MQH	C16-C15	2.07	1.55	1.52
62	z	402	MQH	C55-N56	2.01	1.50	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	z	402	MQH	C34-S35-C31	12.47	97.54	89.70
62	z	402	MQH	S35-C31-N32	-7.95	106.45	114.22
61	z	401	GDP	C5-C4-N3	-5.61	119.46	128.39
62	z	402	MQH	C05-C04-C09	-5.26	106.77	113.04
61	z	401	GDP	C2-N3-C4	4.87	120.69	112.30
62	z	402	MQH	C12-C11-N10	-4.87	102.42	111.22
62	z	402	MQH	C33-C34-S35	-4.22	104.89	110.27
62	z	402	MQH	O28-C27-C26	4.01	120.12	111.47
62	z	402	MQH	C25-C31-S35	3.95	127.05	121.79
61	z	401	GDP	C6-C5-N7	3.90	137.38	130.29
61	z	401	GDP	N9-C4-N3	3.68	133.31	125.95
62	z	402	MQH	C33-N32-C31	3.62	116.74	109.86
62	z	402	MQH	C48-N53-C54	3.51	121.44	118.50
62	z	402	MQH	C11-C12-N13	3.18	119.77	115.69
61	z	401	GDP	C4-C5-N7	-2.92	106.05	110.67
62	z	402	MQH	C04-C09-N56	2.83	124.46	115.99
62	z	402	MQH	C09-C04-N03	2.58	112.54	108.14
62	z	402	MQH	C48-C47-N46	2.40	119.91	115.59
62	z	402	MQH	C54-C55-N56	-2.30	105.23	110.90
62	z	402	MQH	O37-C12-N13	-2.24	118.96	122.96
62	z	402	MQH	C47-C48-N53	-2.20	106.93	112.01
62	z	402	MQH	C49-C48-C47	2.15	115.67	111.04
62	z	402	MQH	O01-C02-N03	-2.11	119.19	122.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	z	401	GDP	PA-O3A-PB-O3B

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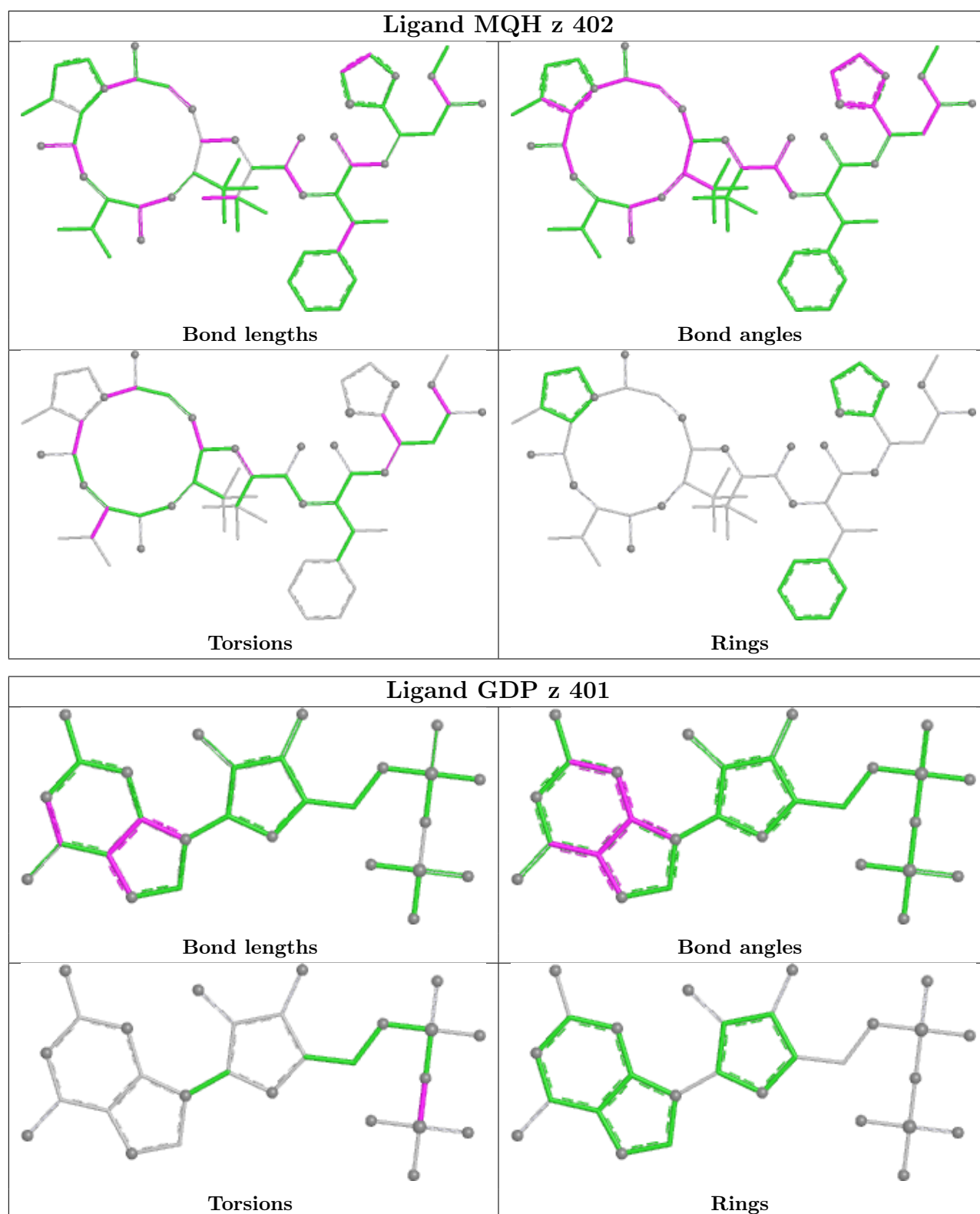
Mol	Chain	Res	Type	Atoms
62	z	402	MQH	C38-C11-N10-C09
62	z	402	MQH	C31-C25-N24-C23
62	z	402	MQH	C26-C27-O28-C29
62	z	402	MQH	N46-C47-C48-C49
62	z	402	MQH	O58-C47-C48-C49
62	z	402	MQH	C55-C54-N53-C48
62	z	402	MQH	O30-C27-O28-C29
62	z	402	MQH	N46-C42-C43-C45
62	z	402	MQH	C04-C09-N56-C55
62	z	402	MQH	C02-C42-C43-C45
62	z	402	MQH	C02-C42-C43-C44
62	z	402	MQH	N46-C42-C43-C44
62	z	402	MQH	N46-C47-C48-N53
62	z	402	MQH	O58-C47-C48-N53
62	z	402	MQH	N10-C09-N56-C55
62	z	402	MQH	C26-C25-N24-C23
62	z	402	MQH	N24-C25-C31-N32
62	z	402	MQH	N24-C25-C31-S35
62	z	402	MQH	C55-C54-N53-C52
61	z	401	GDP	PA-O3A-PB-O2B
61	z	401	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	z	402	MQH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

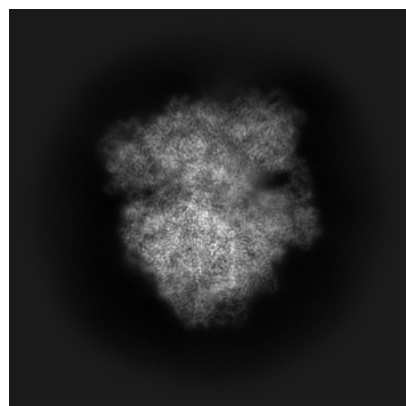
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72204. These allow visual inspection of the internal detail of the map and identification of artifacts.

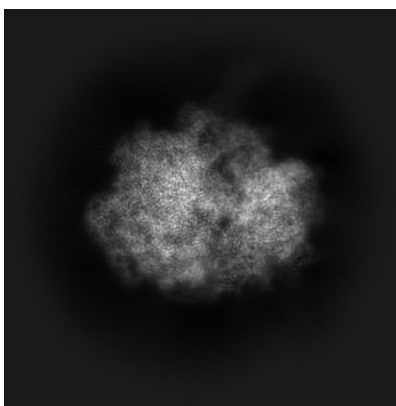
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

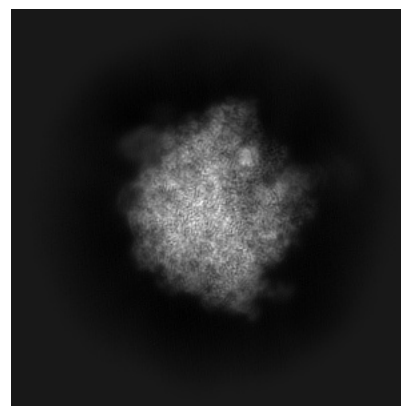
6.1.1 Primary map



X

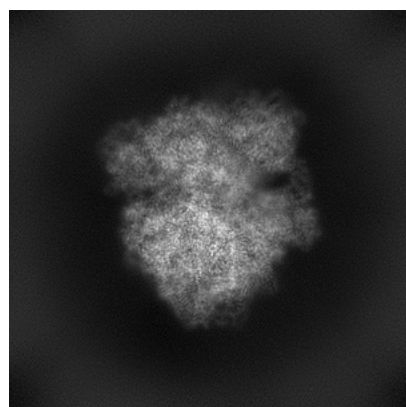


Y

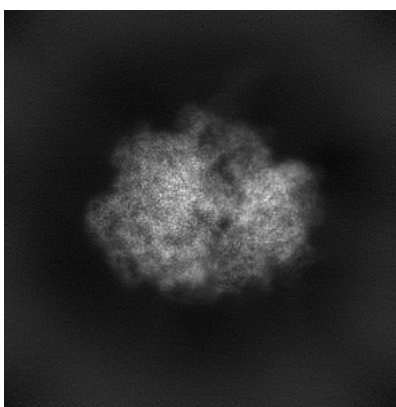


Z

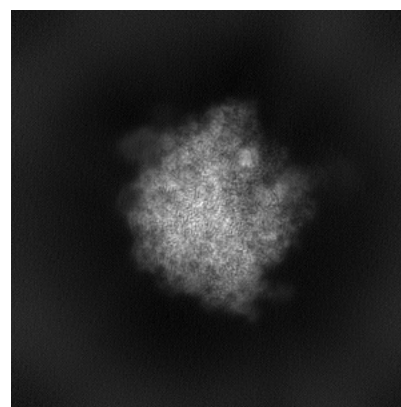
6.1.2 Raw map



X



Y

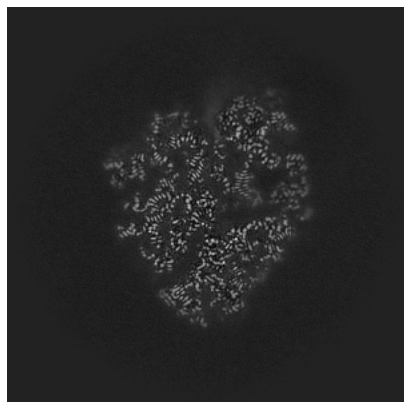


Z

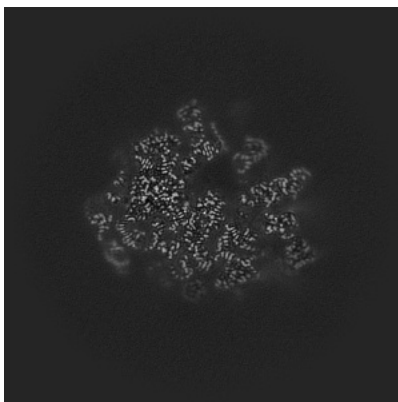
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

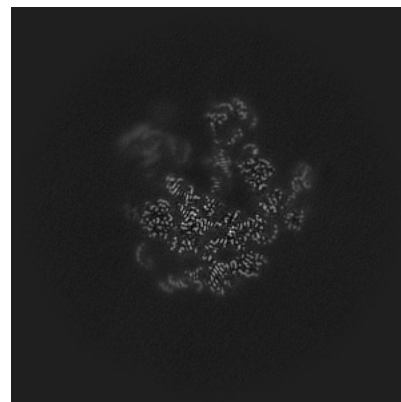
6.2.1 Primary map



X Index: 256

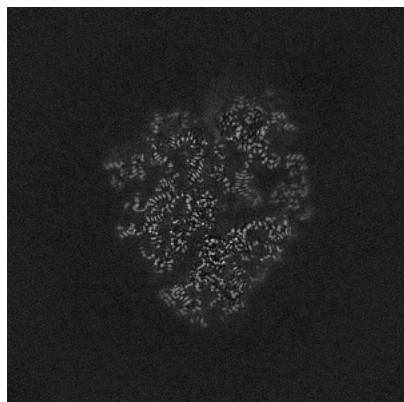


Y Index: 256

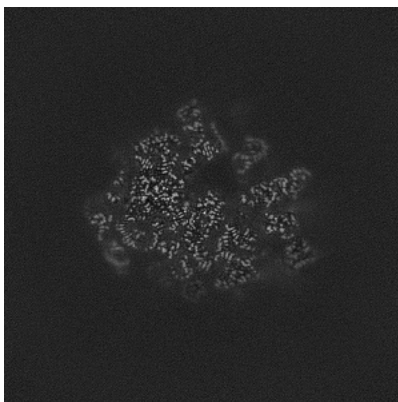


Z Index: 256

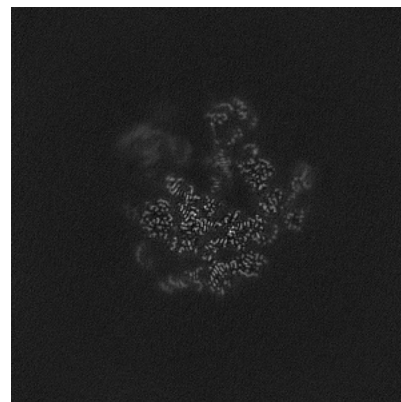
6.2.2 Raw map



X Index: 256



Y Index: 256

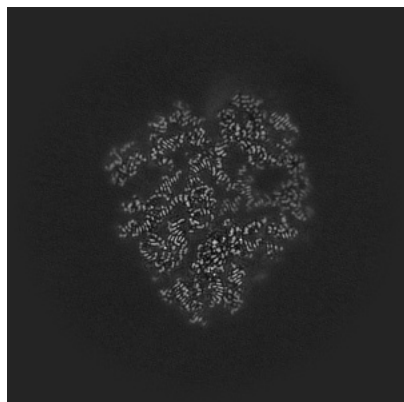


Z Index: 256

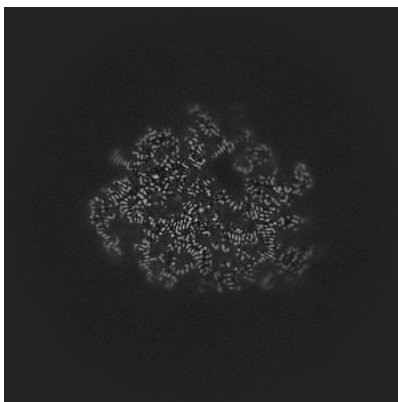
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

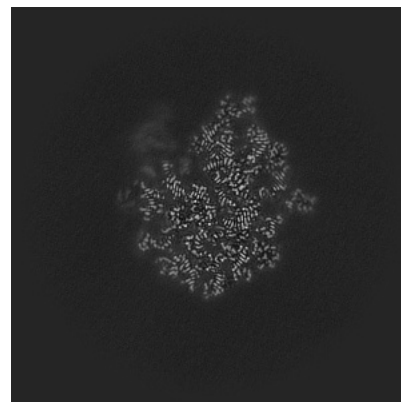
6.3.1 Primary map



X Index: 260

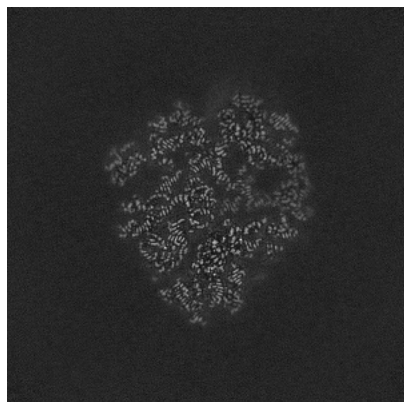


Y Index: 244

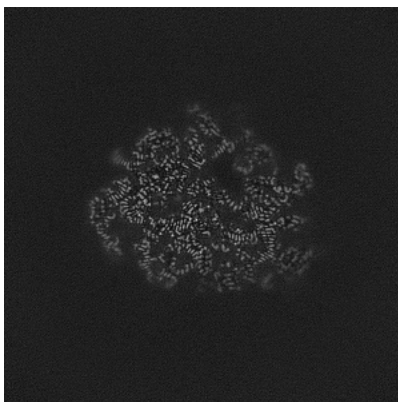


Z Index: 231

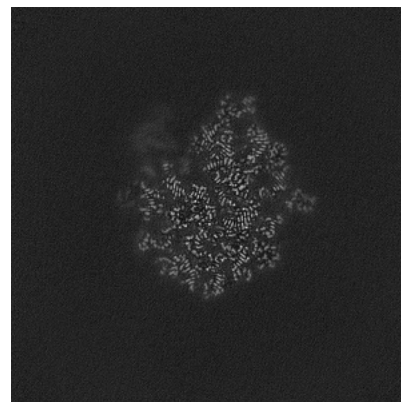
6.3.2 Raw map



X Index: 260



Y Index: 244

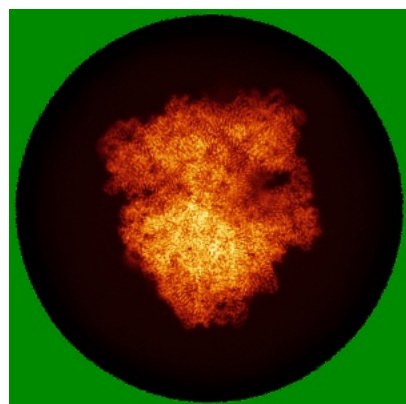


Z Index: 231

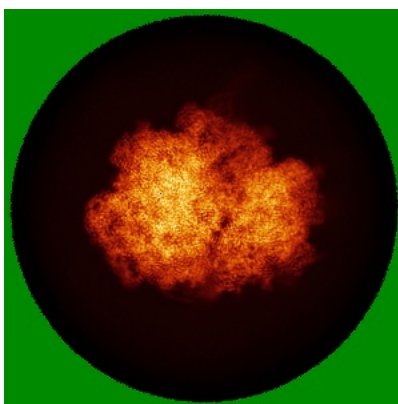
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

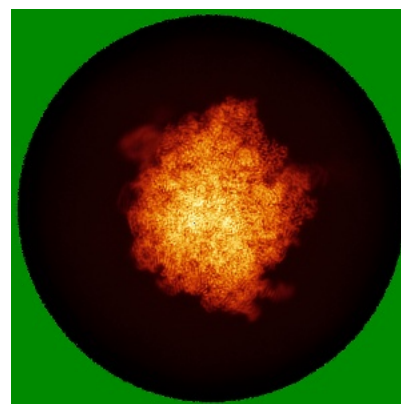
6.4.1 Primary map



X

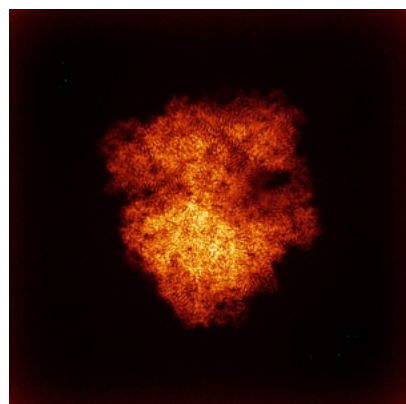


Y

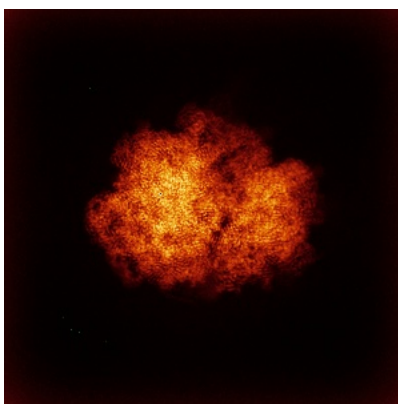


Z

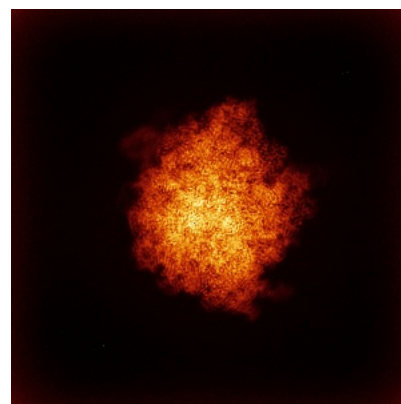
6.4.2 Raw map



X



Y

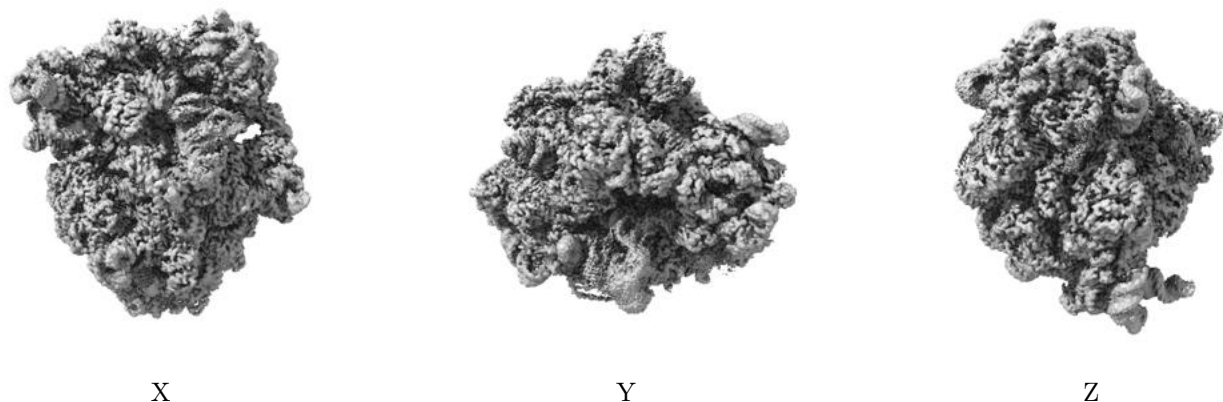


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

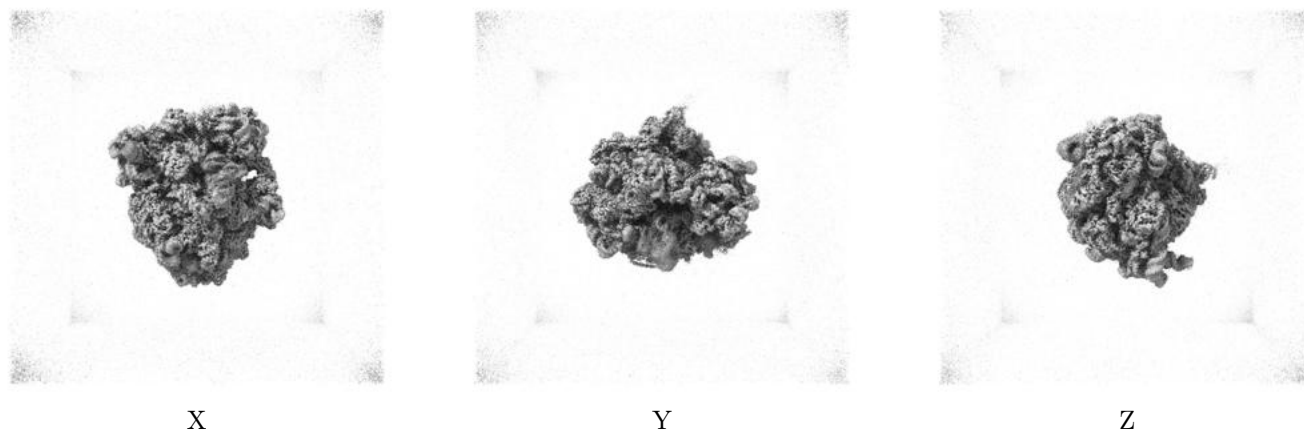
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

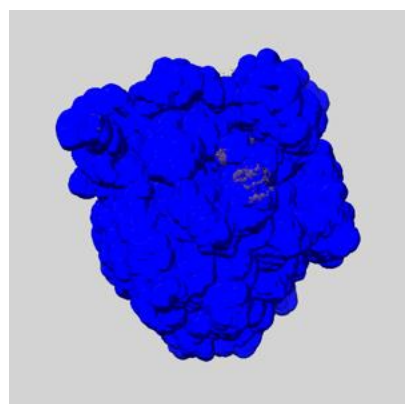
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

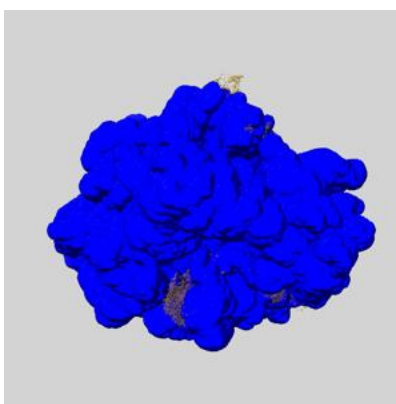
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

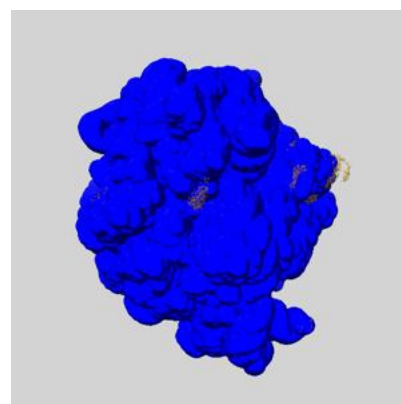
6.6.1 emd_72204_msk_1.map [i](#)



X



Y

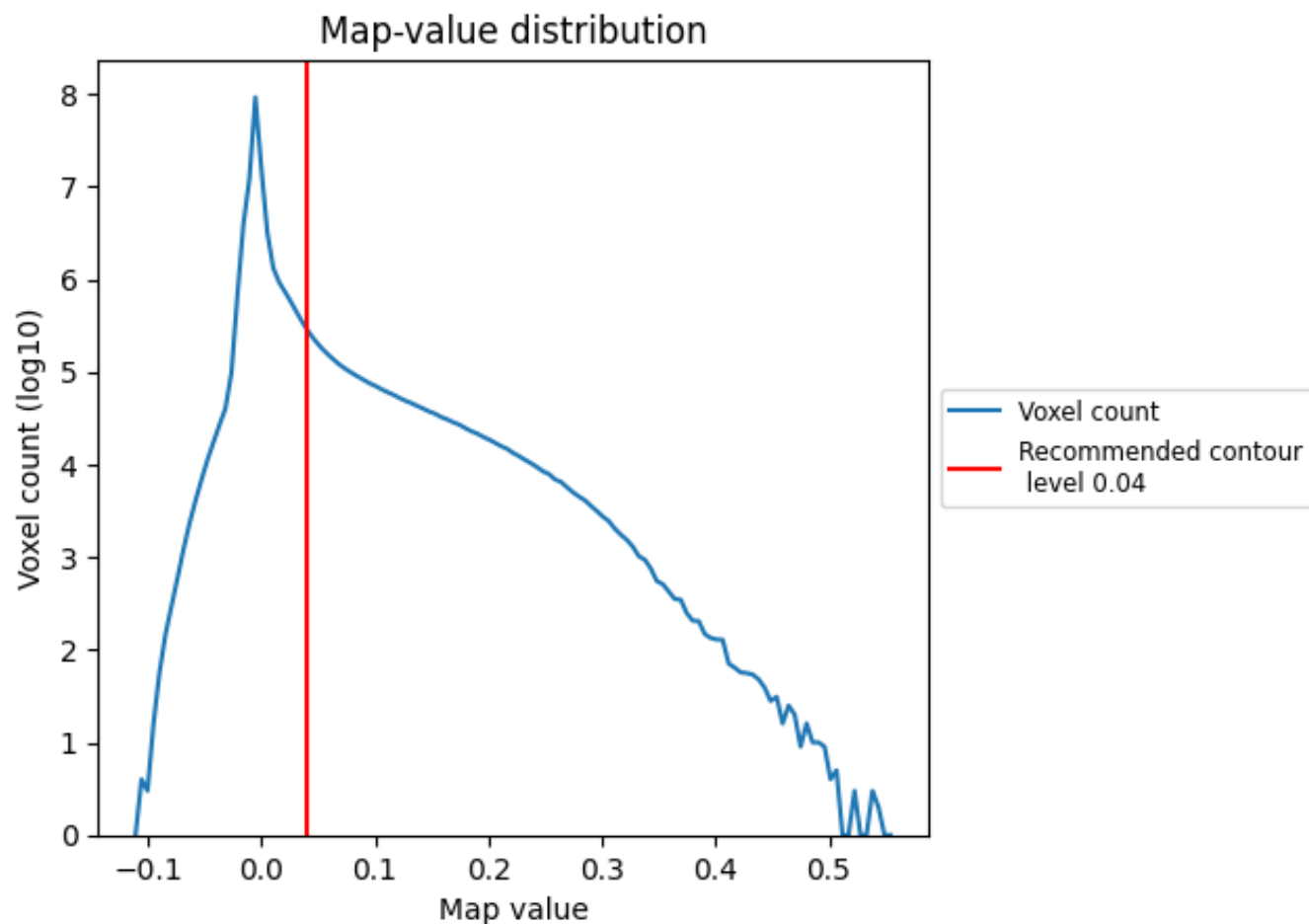


Z

7 Map analysis [i](#)

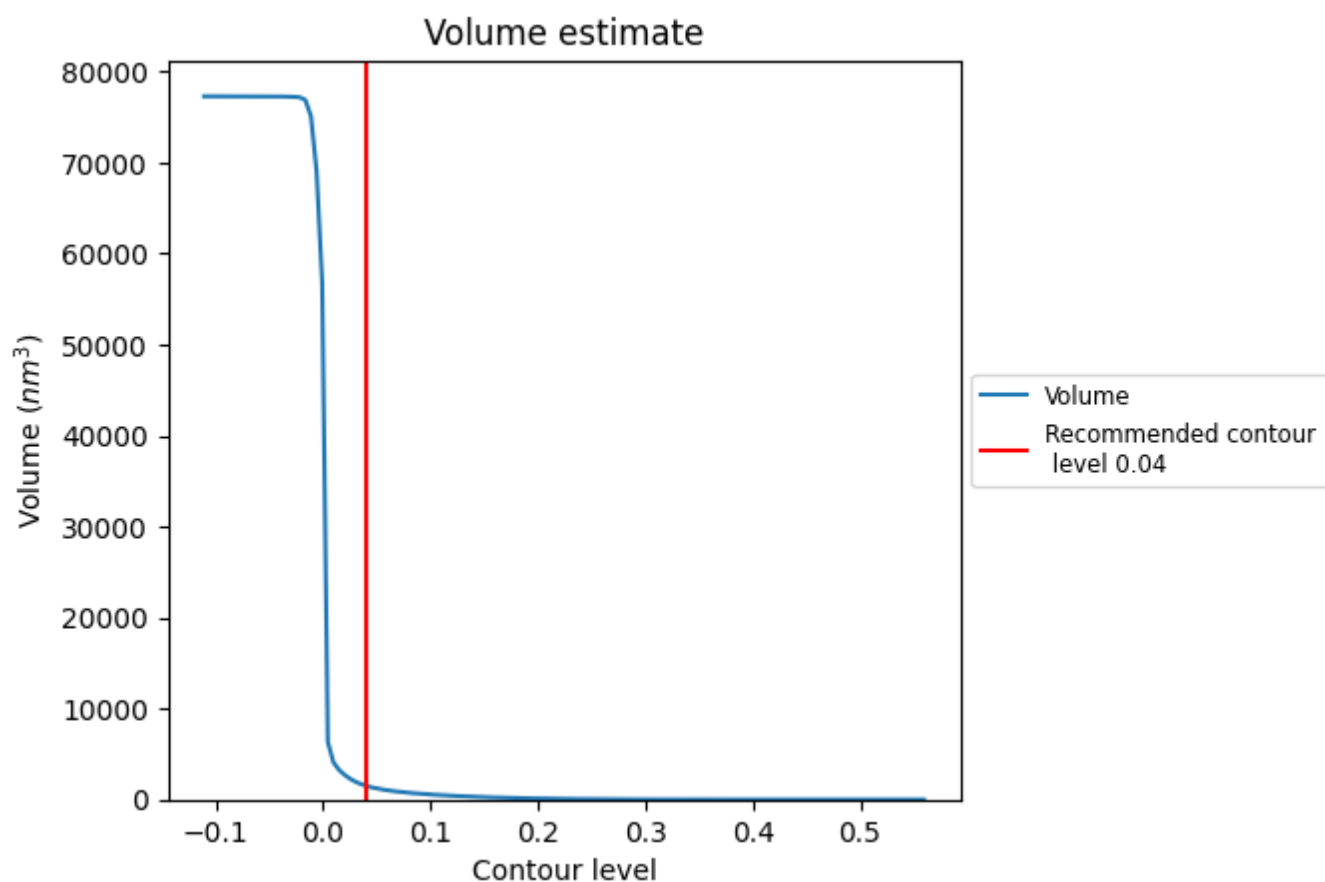
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

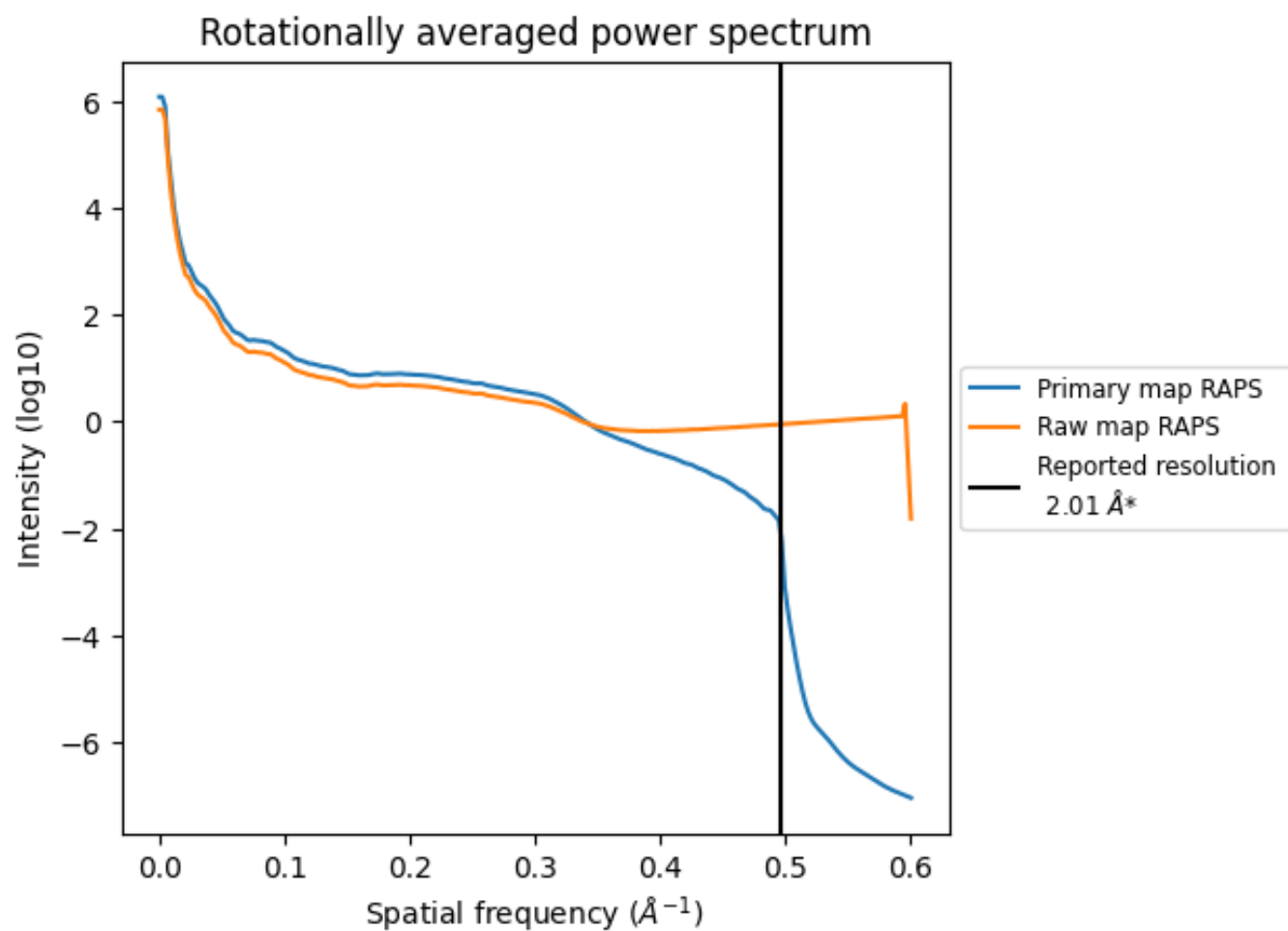
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1512 nm³; this corresponds to an approximate mass of 1366 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

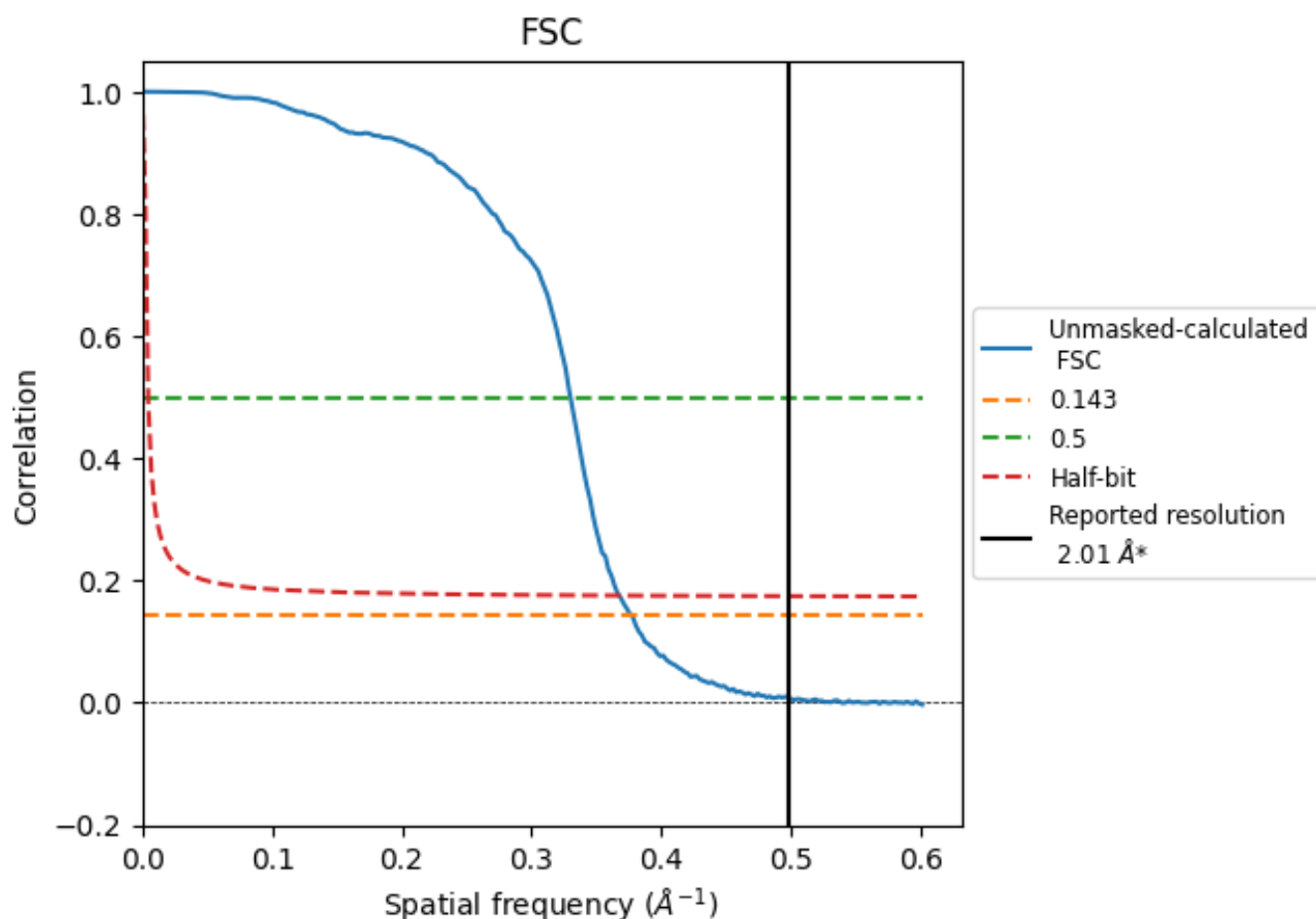


*Reported resolution corresponds to spatial frequency of 0.498 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.498 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

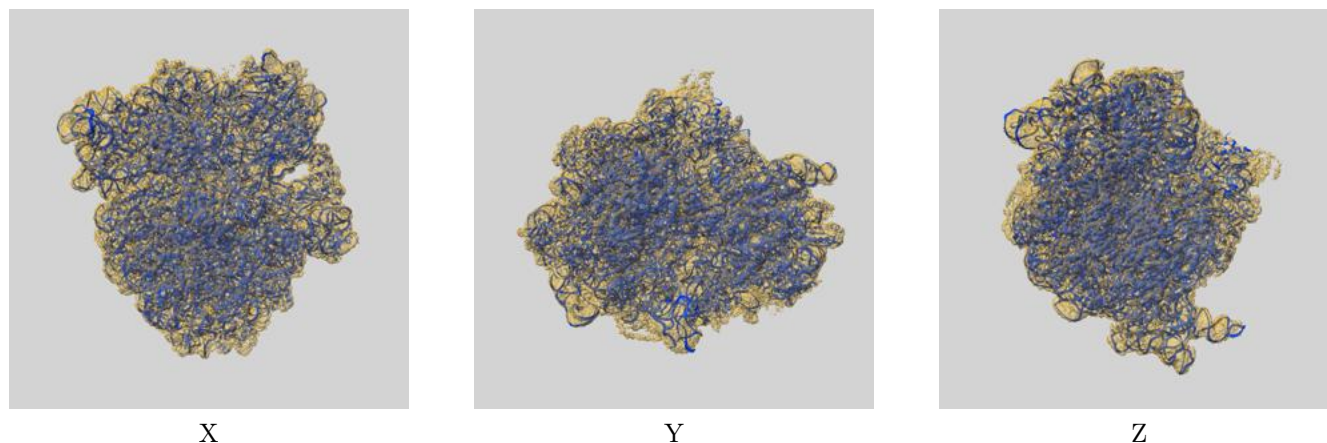
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.65	3.03	2.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.01 by more than 10 %

9 Map-model fit [i](#)

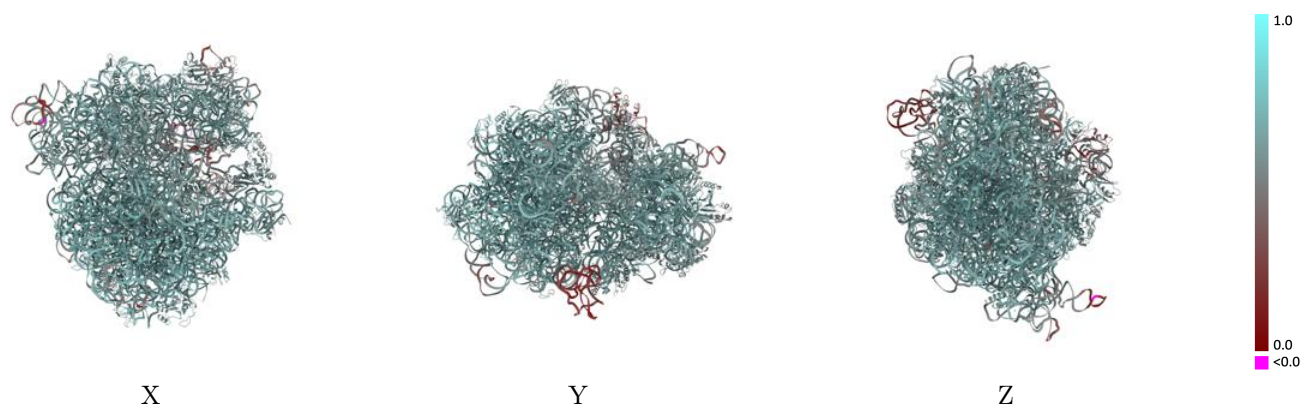
This section contains information regarding the fit between EMDB map EMD-72204 and PDB model 9Q3Q. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



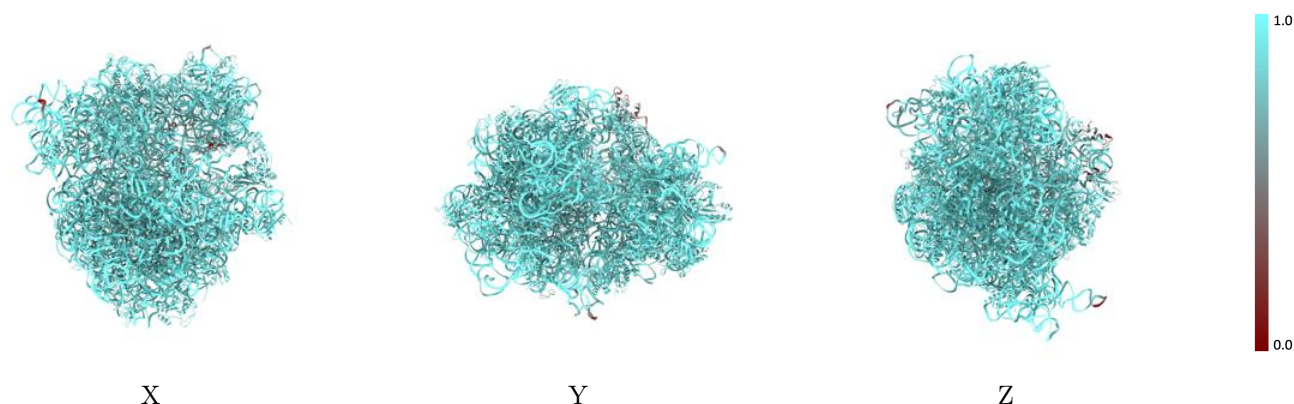
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



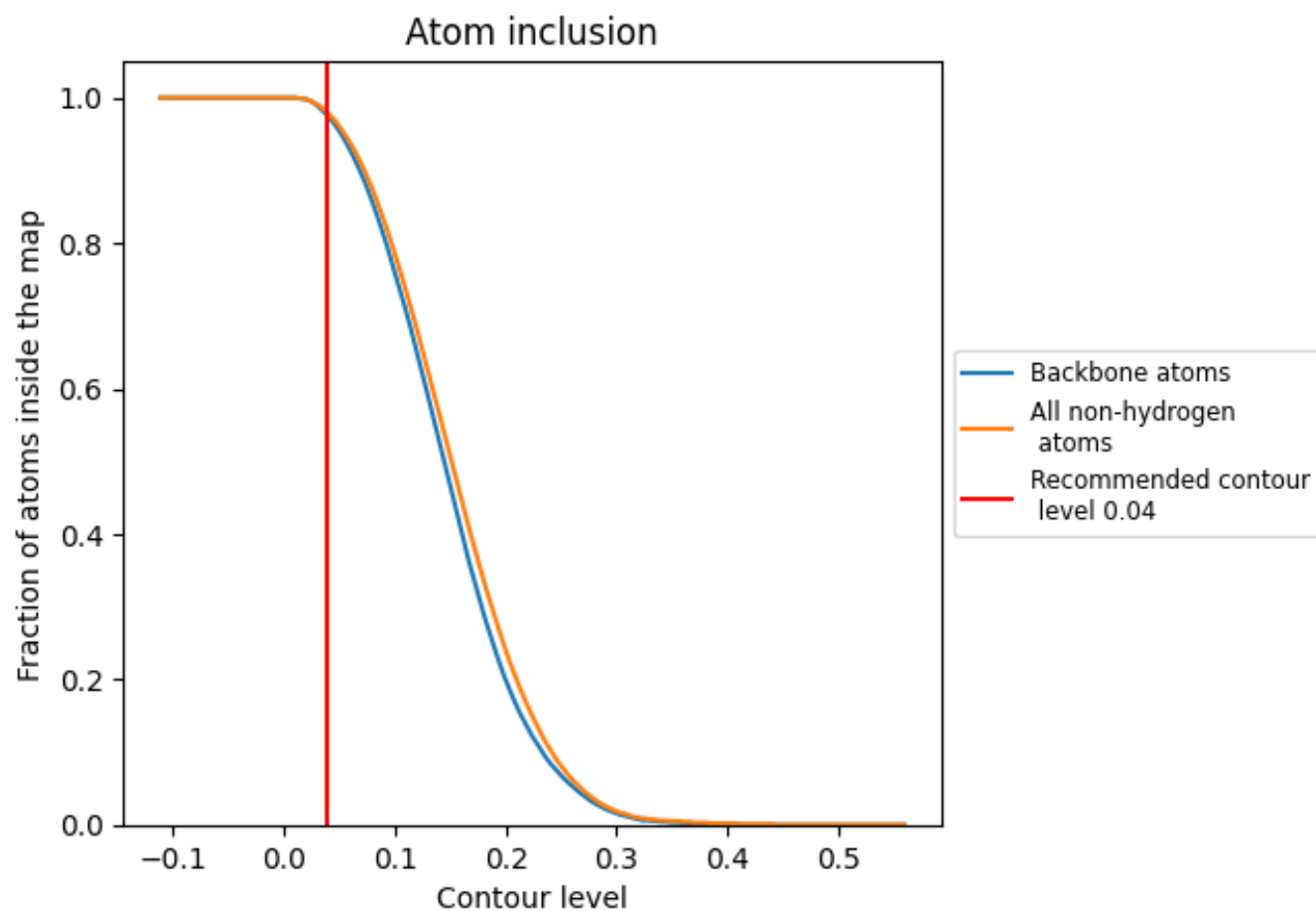
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9790	 0.6390
1	 0.9590	 0.5990
2	 0.9590	 0.6650
3	 0.9320	 0.5500
4	 0.9910	 0.6820
5	 0.9510	 0.6500
6	 0.9970	 0.7120
7	 0.9880	 0.6870
8	 0.9860	 0.6680
A	 0.9910	 0.6480
B	 0.9950	 0.6170
C	 0.9910	 0.6910
D	 0.9710	 0.6790
E	 0.9600	 0.6500
F	 0.9400	 0.5890
G	 0.9450	 0.5840
H	 0.8200	 0.5660
J	 0.5660	 0.3490
L	 0.9830	 0.6730
M	 0.9770	 0.6770
N	 0.9790	 0.6680
O	 0.9750	 0.6730
P	 0.9950	 0.6910
Q	 0.9580	 0.6130
R	 0.9630	 0.6700
S	 0.9930	 0.6940
T	 0.9570	 0.6570
U	 0.9710	 0.6780
V	 0.9500	 0.6490
W	 0.9640	 0.6220
X	 0.9470	 0.6350
Y	 0.9790	 0.6760
Z	 0.9800	 0.6650
a	 0.9920	 0.6370
b	 0.9000	 0.5740



Continued on next page...

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Chain	Atom inclusion	Q-score
c	 0.9580	 0.6320
d	 0.9590	 0.6230
e	 0.9710	 0.6530
f	 0.9440	 0.5930
g	 0.9390	 0.5920
h	 0.9650	 0.6510
i	 0.9530	 0.6160
j	 0.9110	 0.5730
k	 0.9700	 0.6340
l	 0.9880	 0.6810
m	 0.9640	 0.6140
n	 0.9720	 0.6300
o	 0.9680	 0.6320
p	 0.9690	 0.6340
q	 0.9700	 0.6390
r	 0.9650	 0.6250
s	 0.9550	 0.6070
t	 0.9710	 0.6210
u	 0.9180	 0.5690
v	 0.9920	 0.6430
w	 0.9810	 0.5770
x	 0.9840	 0.6140
y	 0.9310	 0.5830
z	 0.9390	 0.5870